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Structures of some hydrated rare earth ethylsulfates

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STRUCTURES OF SOME HYDRATED RARE EARTH ETHYLSULFATES

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I. INTRODUCTION

A. Structural Interest

1. Crystalline fields and spectra

The spectra arising from an ion in a crystal are usually composed of diffuse lines or bands. The reason for this is the strong perturbation of the energy levels of the ion by the instantaneous crystalline field.

The rare earth ions in a crystal, having 4f electrons shielded from field fluctuations by a closed 5 s^2p^6 shell, give sharp spectra. An averaged field does penetrate and cause splitting and shifting of the ions' 4f energy levels. Consequently, these spectra contain information about the crystalline field, and the electronic structure of the ion. If the electronic structure of the ion is known, the crystalline fields can be studied. The splitting of degenerate energy levels and the transition selection rules are dependent upon the field symmetry about the ion. Such an analysis has been made for europium ethylsulfate nonahydrate by E. V. Sayre and S. Freed (1). The symmetry about the rare earth ion used in this investigation was D_{3h} for the water molecules and C_{3h} for the complete environment. These symmetries were obtained from the work of J. A. A. Ketelaar which will be discussed later in this chapter.

The paramagnetic resonance spectra of gadolinium and neodymium ethylsulfates have been studied by B. Bleaney, H. E. D. Scovil, and R. S. T. Trenam (2). The results are consistent with an ion symmetry of C_{3h} except for some discrepancies in the position of the zero field lines. The origin of these discrepancies is not clear. Work on other magnetic properties of the rare earth salts is being carried out by R. M. Bozorth (3).

Active investigations of the magnetic properties, heat capacities and spectra of the rare earth ethylsulfates are being carried out by F. H. Spedding and co-workers (4). The accurate spectra obtained in this work will enable a careful and thorough analysis of the crystalline field perturbations in the excited as well as in the ground state.

One of the reasons for this present investigation is to furnish an accurate structure for the ethylsulfate compounds so that the symmetry of the water molecules about the rare earth ion will be known. In addition, if field strengths are to be computed, the positions of the sulfate oxygens and the orientation of the water dipoles must be known. This information can be obtained from a careful study of the crystals by X-ray diffraction.

2. The Jahn-Teller effect

It was shown by H. A. Jahn and E. Teller (5) that a configuration of a polyatomic molecule for an electronic state having orbital degeneracy cannot be stable with respect to all displacements of the nuclei unless, in the original configuration, the nuclei all lie on a straight line. If electronic spin degeneracy is also included (6), the degenerate nonlinear configuration can be stable only if the degeneracy is of the Kramers type (7), which can occur only if the molecule contains an odd number of electrons. Consequently, the stable state of such a system must be asymmetric enough to split the degeneracy of the ground state.

The structures of the titanium and vanadium alums were discussed by J. H. VanVleck (8), (9) and the size of the distortions of the coordinated water molecules produced by the Jahn-Teller effect was predicted to be about 10^{-9} cm. The distortions which would be expected in the case of the rare earth ions were predicted to be about 10^{-11} cm. Such differences could be detected in the case of the alums but the distortions expected for the rare earth compounds are too small to be detected at the present state of the art of X-ray diffraction. However, a careful structure determination would place an upper limit on such distortions and could verify experimentally that the distortions were indeed quite small.

3. Previous structural investigation

The structures of the rare earth ethylsulfate hydrates have been studied by J. A. A. Ketelaar (10), who determined the lattice constants of many of these compounds with an error of $\pm$ 0.003 Å in a and of $\pm$ 0.01 Å in c. The compounds were found to be isomorphous within experimental error. The most probable space group was given as C_{6h}^2 - $P6_3/m$ with other possible choices of C_6^6 - $P6_3$ and C_{3h}^1 - $P\bar{6}$. A careful discussion of the symmetry about the rare earth ion was given, with the conclusion that the symmetry was almost certainly C_{3h}.

The rare earth ions were found to be in the special position 1/3, 2/3, 1/4 and 2/3, 1/3, 3/4. The sulfur was found to be in a six-fold set with the parameters 0.35, 0.02, 0.25. The sulfate oxygens were assigned to two six-fold sets and one twelve-fold set and approximate parameters were given so as to produce a tetrahedron of oxygens about each sulfur. The parameters of the carbon atoms and water molecules were not given, but, from packing considerations, a structure was postulated. This structure places nine water molecules about the rare earth ion and one of the two six-fold sulfate oxygens in the mirror plane of the rare earth ion at a distance of 2.90 Å.

In view of the available techniques for evaluating structures at that time, it was not practical to continue the structural determination. One of the reasons for the present work is to check and complete the above structural determination.

B. Methods of Computation

1. Computation requirements

The determination of the structure of a moderately complex crystal may require many evaluations of certain Fourier series and a refinement of the model so obtained by the use of a least squares technique.

The Fourier series representing either the electron density or the Patterson function is usually evaluated on a lattice containing from six thousand to five hundred thousand points. The series itself may contain from two hundred to several thousand terms. It can be seen that hand computation is feasible only in the smallest cases and is practically impossible in the more general cases.

The least squares refinement of a moderately complex model may require the fitting of from two hundred to several thousand pieces of data to from twenty to fifty parameters related to the data through a set of trigonometric equations. For small quantities of data and few parameters, hand computation is quite feasible but, in the more extensive cases, the labor and the errors involved in hand computation prohibit the use of the method.

These computations are almost ideally suited for evaluation by large scale digital computers. Because of limitations on the speed and memory capacity of currently available computers, and because the computations must be economically justified, much care must be used in setting up such problems for the computing machines. The method to be used or the form and nature of the answers to be obtained must be adjusted to these demands.

2. The I.B.M. 650

The Type 650 Magnetic Drum Data-Processing Machine manufactured by the International Business Machine Corporation, commonly abbreviated the I.B.M. 650, is a medium sized digital computer using a magnetic drum memory system. This general purpose computer has storage facilities for 2000 "words" on a magnetic drum. Each word is an order or a ten digit number with sign. Each of the 2000 locations is assigned a four digit address of 0000 to 1999. The input and output for the basic machine is in the form of punched cards. For further information please refer to the instruction manual for the I.B.M. 650 (11). The advent of this machine on campus has made it possible to carry out the calculations described above on a routine basis. It is not large enough nor fast enough to handle the very complex crystals but it can handle all moderately complex problems in an economical manner. It should be pointed out that the reasons the very complicated problems are not feasible are essentially economic. A larger machine can carry out such calculations economically. Provided the problems are broken up properly, such calculations can be carried out on the I.B.M. 650 in a matter of a few days if the resulting expense is acceptable.

Many crystallographers have access to this computer and the interest in obtaining crystallographic programs for the I.B.M. 650 is high. Many crystallographic programs have been and are being written and the program library is large enough so that the application of the normal methods of structure analysis becomes almost routine. Information as to the availability of crystallographic programs is available either from the International Business Machines Corporation or from the Computation and Data Processing Center of the University of Pittsburgh.

Since there existed a need for several programs which were not available, it was felt that it would be both interesting and useful to write the required programs. During the course of this work it was found convenient to modify the excellent least squares program, L.S.II (12) which was already available.

The greatest lack of programs seemed to lie in the area of Fourier series evaluation. Consequently, the programming effort was designed to remedy this lack. Because of the limitations of the I.B.M. 650, much thought was given to the problem of adapting the computation method and the form of the output to the I.B.M. 650.

II. COMPUTATIONAL METHODS

A. Evaluation of the Fourier Series

1. General problem

The electron density in the unit cell of a crystal can be represented as a three dimensional Fourier series (13). This series takes the form

$$(1)\quad \rho(x,y,z) = 1/V \sum_{hk\ell\,=\,-\infty}^{\infty} F(hk\ell)\ \exp -2\pi i(hx/a + ky/b + \ell z/c)$$

where $\rho(x,y,z)$ is the electron density, $F(hk\ell)$ is the structure factor for the reflection $(hk\ell)$, V is the volume of the unit cell and a,b,c, are the unit cell dimensions. In the normal case of a mosaic crystal, the intensity of the $(hk\ell)$ reflection is proportional to the square magnitude of the structure factor. All information as to the phase angle of the reflection is lost when the intensity of the reflection is recorded. This information must be recovered by the use of a trial model for the structure, by the use of the Patterson function discussed below, or by some other means. There are some more direct methods for solving the phase problem, but they will not be discussed here. The phase angle calculated on the basis of the trial model can be used to assign a phase angle to the observed magnitudes of $F(hk\ell)$. The series (1) can then be summed. The resulting electron density can be compared with the model used. If the model is correct the electron density will agree except for series termination errors. This error arises from the termination of the series after a finite number of terms. If the electron density does not agree with the model, a new model is required. If, as is usually the case, the electron density agrees with the model in some important features but disagrees or supplements the model in other features, modification of the model and recalculation of the electron density may lead to convergence on the correct model.

The Fourier series, in somewhat different form, may lend more direct assistance in obtaining a suitable model. The function

$$(2)\quad P(x,y,z) = 1/V \sum_{hk\ell \atop -\infty}^{\infty} |F(hk\ell)|^2 \exp -2\pi i(hx/a + ky/b + \ell z/c)$$

which uses only coefficients which are directly related to the observed intensities is known as the Patterson function (14). This function can be interpreted as having a maximum at those points which correspond to the end point of some interatomic vector referred to the origin of the unit cell. Because of the large number of such maxima, this function rarely can be interpreted to give a complete model. In many cases, however, at least some of the more important features of the model can be obtained. The problem of the evaluation of such series is essentially the same as the problem of the evaluation of the electron density function.

The above discussion is not intended to be complete. There are other techniques utilizing Fourier series which are useful, but which involve the same computational problem.

If the wave length of the X-radiation is not too close to an absorption edge of a crystal component, Freidel's law (15), which states that $F(hk\ell)$ is the conjugate of $F(\bar{h}\bar{k}\bar{\ell})$, will hold. The notation $\bar{h}\bar{k}\bar{\ell}$ means $-h$, $-k$, and $-\ell$. By using the expressions $F(hk\ell) = A(hk\ell) + iB(hk\ell) = F^{*}(\bar{h}\bar{k}\bar{\ell}) = A(\bar{h}\bar{k}\bar{\ell}) - iB(\bar{h}\bar{k}\bar{\ell})$ and $\theta(hk\ell) = 2\pi(hx/a + ky/b + \ell z/c)$ the electron density can be written as

$$
\begin{aligned}
(3)\ \rho(x,y,z) = 2/V \sum_{hk\ell\,1}^{\infty} \Big[& A(hk\ell)\cos\theta(hk\ell) + B(hk\ell)\sin\theta(hk\ell) \\
& + A(\bar{h}\bar{k}\ell)\cos\theta(\bar{h}\bar{k}\ell) + B(\bar{h}\bar{k}\ell)\sin\theta(\bar{h}\bar{k}\ell) \\
& + A(h\bar{k}\ell)\cos\theta(h\bar{k}\ell) + B(h\bar{k}\ell)\sin\theta(h\bar{k}\ell) \\
& + A(\bar{h}k\ell)\cos\theta(\bar{h}k\ell) + B(\bar{h}k\ell)\sin\theta(\bar{h}k\ell) \Big] \\
+ 2/V \sum_{k\ell\,1}^{\infty} \Big[& A(0k\ell)\cos\theta(0k\ell) + B(0k\ell)\sin\theta(0k\ell) \\
& + A(0\bar{k}\ell)\cos\theta(0\bar{k}\ell) + B(0\bar{k}\ell)\sin\theta(0\bar{k}\ell) \Big] \\
+ 2/V \sum_{h\ell\,1}^{\infty} \Big[& A(h0\ell)\cos\theta(h0\ell) + B(h0\ell)\sin\theta(h0\ell) \\
& + A(\bar{h}0\ell)\cos\theta(\bar{h}0\ell) + B(\bar{h}0\ell)\sin\theta(\bar{h}0\ell) \Big]
\end{aligned}
$$

$$+ 2/V \sum_{\substack{hk\\1}}^{\infty} \left[A(hk0) \cos \theta(hk0) + B(hk0) \sin \theta(hk0) + A(h\bar{k}0) \cos \theta(h\bar{k}0) + B(h\bar{k}0) \sin \theta(h\bar{k}0)\right]$$

$$+ 2/V \sum_{\substack{h\\1}}^{\infty} \left[A(h00) \cos \theta(h00) + B(h00) \sin \theta(h00)\right]$$

$$+ 2/V \sum_{\substack{k\\1}}^{\infty} \left[A(0k0) \cos \theta(0k0) + B(0k0) \sin \theta(0k0)\right]$$

$$+ 2/V \sum_{\substack{\ell\\1}}^{\infty} \left[A(00\ell) \cos \theta(00\ell) + B(00\ell) \sin \theta(00\ell)\right]$$

$$+ 1/V\ A(000).$$

This particular expression is derived in a form containing only positive values of ℓ for convenience in adapting to the I.B.M. 650 program.

If we include the special reflections (those containing one or more zero indices) in the general form, they must be divided by a multiplicity factor of 2^N where N is the number of zero indices occurring in $F(hk\ell)$. If we define $F'(hk\ell) = \frac{2^{1-N}}{V} F(hk\ell)$, the summation now becomes

$$(4)\ \rho(x,y,z) = \sum_{hk\ell}^{\infty}{}_{0} \Big[A'(hk\ell)\cos\theta(hk\ell) + B'(hk\ell)\sin\theta(hk\ell)$$

$$+ A'(\bar{h}\bar{k}\ell)\cos\theta(\bar{h}\bar{k}\ell) + B'(\bar{h}\bar{k}\ell)\sin\theta(\bar{h}\bar{k}\ell)$$

$$+ A'(h\bar{k}\ell)\cos\theta(h\bar{k}\ell) + B'(h\bar{k}\ell)\sin\theta(h\bar{k}\ell)$$

$$+ A'(\bar{h}k\ell)\cos\theta(\bar{h}k\ell) + B'(\bar{h}k\ell)\sin\theta(\bar{h}k\ell)\Big].$$

By using the trigonometric identities,

$$\cos\theta(hk\ell) = \cos\theta(h00)\cos\theta(0k0)\cos\theta(00\ell)$$

$$- \cos\theta(h00)\sin\theta(0k0)\sin\theta(00\ell)$$

$$- \sin\theta(h00)\cos\theta(0k0)\sin\theta(00\ell)$$

$$- \sin\theta(h00)\sin\theta(0k0)\cos\theta(00\ell)$$

and,

$$\sin\theta(hk\ell) = \sin\theta(h00)\cos\theta(0k0)\cos\theta(00\ell)$$

$$+ \cos\theta(h00)\sin\theta(0k0)\cos\theta(00\ell)$$

$$+ \cos\theta(h00)\cos\theta(0k0)\sin\theta(00\ell)$$

$$- \sin\theta(h00)\sin\theta(0k0)\sin\theta(00\ell)$$

the expression for the electron density becomes, in expanded form,

$$(5)\ \rho(x,y,z) = \sum_{hk\ell}^{\infty}{}_{0} \Big[A_1(hk\ell)\cos\theta(h00)\cos\theta(0k0)\cos\theta(00\ell)$$

$$+ A_2(hk\ell)\sin\theta(h00)\sin\theta(0k0)\cos\theta(00\ell)$$

$$+ A_3(hk\ell) \sin \theta(h00) \cos \theta(0k0) \sin \theta(00\ell)$$
$$+ A_4(hk\ell) \cos \theta(h00) \sin \theta(0k0) \sin \theta(00\ell)$$
$$+ B_1(hk\ell) \sin \theta(h00) \sin \theta(0k0) \sin \theta(00\ell)$$
$$+ B_2(hk\ell) \cos \theta(h00) \cos \theta(0k0) \sin \theta(00\ell)$$
$$+ B_3(hk\ell) \cos \theta(h00) \sin \theta(0k0) \cos \theta(00\ell)$$
$$+ B_4(hk\ell) \sin \theta(h00) \cos \theta(0k0) \cos \theta(00\ell)\Big] .$$

The A_i and B_i are linear combinations of $A'(hk\ell)$ and $B'(hk\ell)$ respectively.

These expressions are

$$
\begin{aligned}
A_1 &= A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_2 &= -A'(hk\ell) - A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_3 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) - A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\
A_4 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) - A'(\bar{h}k\ell) \\
B_1 &= -B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_2 &= B'(hk\ell) + B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_3 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) - B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\
B_4 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) - B'(\bar{h}k\ell)
\end{aligned}
\tag{6}
$$

The space group of the crystal introduces other symmetry and creates relationships among the $A(hk\ell)$ and the $B(hk\ell)$ that usually simplify the above expressions. It should be noted that, if the space group possesses a center of symmetry, $F(hk\ell) = F(\bar{h}\bar{k}\bar{\ell})$. But Friedel's Law states that $F(hk\ell) = F^*(\bar{h}\bar{k}\bar{\ell})$, and so we must have all $B(hk\ell) = 0$.

There are two general methods for evaluating such series; one is to evaluate the series directly as a three dimensional sum in the form (4) or (5), the other is to use form (5) and to evaluate it as successive one dimensional summations. In general, it can be said that the calculation time required for successive one dimensional summations is relatively independent of the number of terms to be summed provided the symmetry is unchanged, while the direct evaluation is essentially proportional to the number of terms to be summed. The intermediate results which must be retained are much more extensive in the first case than in the second. It can be seen that the best form is strongly dependent upon the specifications of the computer to be used and the number of terms to be considered. In general, provided the requirements for moderately fast large capacity storage can be met, it would appear better to do full calculations in the expanded form and partial calculations of correction terms in the unexpanded form. The correction results could be added to the previous results to give the new function.

Another point, which is of great interest, is the possibility of evaluating such series only over the basic 1/64 of the unit cell (1/4 x 1/4 x 1/4). Use can be made of trigonometric relationships to produce the required values in the remainder of the cell. In the case of series (4) this involves breaking the calculation up into groups of terms, each of which transform in the same way. The sums of each group can then be transformed to give the final result. Unfortunately, this requires a knowledge of the same expression with sin substituted for cos and vice versa. This doubling of work is somewhat unsatisfactory and increases the output data. In addition, the translation of these groups is not very simple. Expansion in each of the three dimensions involves such relations as

$$\begin{aligned}\cos(A + m\pi/2) &= \quad \cos A \text{ if } m = 4n \\ &= -\sin A \text{ if } m = 4n + 1 \\ &= -\cos A \text{ if } m = 4n + 2 \\ &= \quad \sin A \text{ if } m = 4n + 3\end{aligned}$$

and

$$\begin{aligned}\sin(A + m\pi/2) &= \quad \sin A \text{ if } m = 4n \\ &= \quad \cos A \text{ if } m = 4n + 1 \\ &= -\sin A \text{ if } m = 4n + 2 \\ &= -\cos A \text{ if } m = 4n + 3\end{aligned}$$

The series (5) can be transformed in a somewhat simpler manner by the relations

$$\begin{array}{ll}\cos 2\pi hx = \cos 2\pi hx & \sin 2\pi hx = \sin 2\pi hx \\ \cos 2\pi h(x+1/4)=(-1)^h\cos 2\pi hx' & \sin 2\pi h(x+1/4)=(-1)^{h+1}\sin 2\pi hx' \\ \cos 2\pi h(x+1/2)=(-1)^h\cos 2\pi hx & \sin 2\pi h(x+1/2)=(-1)^h\sin 2\pi hx \\ \cos 2\pi h(x+3/4)=\cos 2\pi hx' & \sin 2\pi h(x+3/4)= -\sin 2\pi hx'\end{array}$$

where $x' = 1/4 - x$. In the case of an expansion by 1/4 or 3/4, the coordinate corresponding to x in the basic 1/64 of the cell is read in reverse and translated. This is carried out by simply changing the labeling of the points on the final tabulated results.

As a consequence, if the terms of the series are broken up into groups, each with the same translation properties in three dimensions, and the group sums are obtained over the basic 1/64 of the unit cell, the results for the remainder of the cell may be obtained by summing the same groups but with the signs of certain groups changed. This can be carried out automatically at the time of tabulation, even on the I.B.M. 402 tabulator. The proper wiring for any given translation can be selected by three external switches, each controlling the translation in one of the three dimensions. The results of the three independent translations are combined by the use of coselectors to control the addition or subtraction of a given group under the translations set in the switches.

A similar method could be used to expand the results from series (4) but the added complication of having sin and cos type contributions which must be selected would prohibit its use with the I.B.M. 402 tabulator unless these were selected before each translation. The two systems would not be compatible and could not be summed and translated together. Compatibility might be attainable on an I.B.M. 407

tabulator but this has not been investigated. However, if the form (4) is to be used for correction terms only, the most convenient thing to do would probably be to evaluate directly over all of the cell that is of interest. Then if the results were treated as even cos terms, and odd quarters of the unit cell punched in reverse, the corresponding sums for each translation could be added to the original series (5) cards to give the new evaluation of the electron density.

The above treatment of correction terms from series (4) is the most efficient over the basic 1/64 of the unit cell, but duplication becomes comparatively expensive if many such cell fractions must be used. A third procedure, better adapted for many cell fractions but less efficient in the basic 1/64 of the unit cell, is to use series (5) but not to use successive one dimensional summations. By taking advantage of the smaller number of terms, even moderate storage facilities will enable the direct evaluation of the same sub-series and the utilization of the same expansion scheme as for the successive one dimensional summations.

There remains one further question to be discussed. That is the question of the nature of the desired final information and the effect of this on the programming. The Fourier series are used both in searching for new features to be included in a model and in improving the parameters of a rough but essentially complete model. In the first case the volume of the unit cell must be completely explored. In the second case, because of a knowledge of the rough parameters, only a small part of the total unit cell volume really needs to be explored. The three successive one dimensional summations are more suitable for the first case, while small parts of the unit cell can readily be explored by series (4) or by the method discussed above using series (5) without successive summations.

The information in the second case that is really desired is the location of the maximum and the shape of the peak. The results of a limited exploration about the maxima could then be used in a separate program to produce this information. The lattice points must be close enough to accurately define the shape of the peak.

There are three general ways to explore the whole unit cell. One is to evaluate the series on a mesh fine enough to give a satisfactory definition of the peak. The second is to use a rough 'searching' mesh and a fine mesh about each interesting point. The third method is to compute the projection of the electron density onto a plane and then evaluate the electron density along a line perpendicular to each maximum to find the third coordinate. A fine mesh evaluation about this point would then give the desired information.
It would appear that, in any given problem, one of the above procedures would be better than any of the others and that, ideally, one would like to be able to use that method which is thought to be best suited. This would probably require

several different programs. If sufficient storage is available it should be possible to put out only the parameters of the maximum and of the peak shape. This would be easier to do in the second and third cases. The first case, except for enormous storage facilities, would require human selection of points to be used in defining the peak. These could then be fed back into the computer to determine peak parameters.

The use of the various techniques above would require several different programs, some of which are but poorly adapted to evaluation of the basic I.B.M. 650 machine. The advent of faster and larger computational machinery on campus will make most of the above techniques feasible. The following is a discussion of the programs which were written for the I.B.M. 650 as a start toward meeting the above needs.

2. Three dimensional block program

The first attempt to write an I.B.M. 650 program was to carry out the direct summation of series (4) over the basic 1/64 of the unit cell and then to expand to obtain the remainder of the unit cell. It was felt that the avoidance of the large quantities of intermediate data required by successive one dimensional summations would make up the difference in the efficiency of the approach. As mentioned before, the time required is, for series (4), directly proportional to the number of terms considered, while the time required by the one dimensional summations is somewhat independent of the number of terms provided the number of terms is much less than the number of mesh points to be evaluated. Consequently, there must be some point at which the latter method becomes superior. This point was not an easy thing to decide in advance. The actual programming of the direct evaluation led to the conclusion that even for large two dimensional projections the latter method is superior, at least on the basic I.B.M. 650. This latter method subsequently found realization in the T.D.F. 40-80 program which will be discussed in the next section.

One of the things which had promoted so much interest in the direct method was the invention of a subroutine that could obtain, and store for future use, values of cos $\theta(hk\ell)$ or sin $\theta(hk\ell)$ evaluated along a line in the mesh. The time required, aside from initialization for the specific line, was one revolution of the drum per point in the line. This subroutine was so fast that it was hoped that the calculation by this method would make direct evaluation feasible. The use of the unexpanded form (4) is not feasible in general as was discussed above. However, if the number of terms involved or if the number of points involved are small, this procedure has many advantages, including that of speed. Consequently the unexpanded form is good for the evaluation of the electron density about a single maximum. Since, as was discussed, the three dimensional block evaluation is a very useful tool it was decided to write such a program. To save more time, it was decided to open up the interior loops and write them out explicitly. Because of the increased initialization, this did not turn out to be a very good idea, and if the program were to be rewritten, this should not be done. Even so, the final program is quite satisfactory.

The overall design of the program having been carried out, the program was written in collaboration with Mrs. Phyllis A. Keys.

Since there is no need for expansion to other parts of the unit cell in such a program, subseries sums are not required. The summation is by a direct three dimensional procedure and so one pass of the coefficient cards produces a small set of output cards containing the values of the electron density. The values obtained are on the mesh points of a cube of 4 points to a side, that is, a total of 64 points. The mesh points are at such a spacing that there are 80 mesh points along each side of the unit cell. It was felt that this would be enough to define the peaks except possibly for very large cells. If the program were rewritten with uncut loops, it may be that more points could be accommodated. The program computes at a rate of approximately twenty reflections per minute. For a detailed description of the program and a set of operating instructions, please refer to Appendix A.

3. Block peak program

In accordance with the general discussion, it was felt that a program which could take the results of the three dimensional block program and generate a set of parameters describing the peak would be desirable. The procedure is to fit the electron density near the center of a peak using the function

$$\rho = \exp\left[a_0 + a_1x^2 + a_2y^2 + a_3z^2 + a_4x + a_5y + a_6z + a_7yz + a_8xz + a_9xy\right]$$

by means of a least squares treatment. This program was written by Mr. Donald E. Williams and is included here only to complete the discussion of this type of approach. The program was written in the Bell Laboratories interpretive routine and is quite rapid. About one minute is required for each peak. This program has been written up and is available from Mr. Williams (16). This program and the preceding block program are very useful during a refinement of a structure.

4. The T.D.F. 40-80 program

If the model is not firmly established, a complete search of the unit cell is needed. This may be accomplished either by rough scanning and using the block program about maxima or by evaluation of all points on a fine mesh. It was found possible to write a program that could do either job. A mesh of $40 \times 40 \times 40$ points is used for rough scanning and a mesh of $80 \times 80 \times 80$ points is used when all points and a fine mesh are desired. The procedure is based on series (5).

The method of calculation is quite simple and involves the use of two trigonometric tables containing $\cos 2\pi hx$ and $\sin 2\pi hx$ for $h = 1,2,\ldots,39$ and $80\ x = 1,2,\ldots,19$. These values correspond to the 80 mesh program. They are reduced appropriately for the 40 mesh program. The functions are stored with rounded six significant figure accuracy. These tables occupy most of the drum storage. The special values not included above are computed by the program.

A one dimensional summation is evaluated for each pass of the cards. The output cards are then sorted and passed through the I.B.M. 650 again for the next sum. The time required for the calculation may be estimated from a card reading rate of approximately 100 cards per minute and a card punching rate of 100 cards per minute for an evaluation on the $80 \times 80 \times 80$ mesh. The last summation punches results with ten points per card. The intermediate sums punch only one point per card. The number of subsums required depends upon the expansions required to cover that portion of the unit cell which is of interest. The card reading rate is much faster for the $40 \times 40 \times 40$ mesh and, of course, the output from each summation is only half that of the output from the 80 x 80 x 80 mesh evaluation. The output punching rate is still 100 cards per minute. The two programs can be mixed to give differing meshes in different directions. This calculation rate is close to the maximum rate at which cards can be read and punched. The calculations are carried out over only 1/4 x 1/4 x 1/4 of the unit cell. The remainder of the cell is obtained by combining the subsums appropriately at the same time the results are printed.

The time required for a calculation by the above method is essentially just that required to read and punch cards at a rate of 100 cards per minute. Any possible increase in speed as a result of reprogramming must come about through a reduction in the number of cards punched and read. It should be noted that the time being referred to is the time on the I.B.M. 650. Some time is required for sorting, but the expense of this is minor. After the T.D.F. 40-80 program was completed, a modification was discovered which effectively reduces the number of cards punched by a factor of from two to eight. This would now bring computation speeds up to a limit set by punching and reading times with actual internal calculations requiring only a minor amount of time. A further advantage of this modification is that sorting is eliminated for two dimensional evaluations and is greatly reduced for three dimensional evaluations. This modification will be made in the near future. Where an I.B.M. 650 with magnetic tape attachment is available, the speed will be increased by a large factor by using this modification. For details of the T.D.F. 40-80 program please refer to Appendix B.

B. Least Squares Method

1. General problem

A least squares method was first applied to the refinement of crystal structures by E. W. Hughes (17). In order to make clear the application of computer methods and the usefulness of the least squares method, a detailed analysis of the method is given below.

The structure factor can be related to the parameters of the atoms in the crystal by

$$(7)\quad F(hk\ell)=\sum_i f_i(hk\ell)\ \exp\left[-B_i\ \sin^2\theta/\lambda^2\right]\exp\ 2\pi i(hx_i+ky_i+\ell z_i)$$

where λ = wave length of the radiation used,

θ = Bragg reflection angle,

B_i = isotropic temperature factor for atom i,

and x_i, y_i, z_i = coordinates of atom i expressed in fractions of the unit cell.

One measure of agreement between a trial model and the observed data is

$$R_3 = \frac{\sum_u w_u (|F_o| - |F_{ct}|)^2}{\sum_u w_u |F_o|^2} \tag{8}$$

where u = index representing all $hk\ell$,

w_u = weighing factor for $u = h,k,\ell$,

$|F_o|$ = observed structure factor magnitude,

and $|F_{ct}|$ = calculated structure factor magnitude for the trial structure.

If the errors in the observed data obey a Gaussian distribution and if there are no errors in the calculation of F_{ct} the minimization of R_3 with respect to the parameters of the structure will lead to a most probable set of values for the parameters. A general discussion of this relationship is given by E. T. Whittaker and G. Robinson (18). If we denote the values of $|F_{ct}|$ based on the most probable structure by $|F_{cT}|$ we can expand $|F_{cT}|$ about $|F_{ct}|$ in a Taylor series and obtain

$$|F_{cT}| = |F_{ct}| + \sum_{i=1}^{m} \Delta x_i F_i + \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \Delta x_j F_{ij} + \cdots \tag{9}$$

where m = total number of parameters,

Δx_i = corrections to be added to the parameters of the trial model,

$F_i = \left.\frac{\partial |F|}{\partial x_i}\right| x_i$ for the trial model,

$$F_{ij} = \frac{\partial^2 |F|}{\partial x_i \partial x_j} \Bigg| \; x_i, \text{ for the trial model.}$$

The function R_3 will be a minimum when the trial structure is the most probable structure. This implies that

$$\frac{\partial}{\partial x_k} \left[\frac{\sum_u w_u (|F_o| - |F_{cT}|)^2}{\sum_u w_u |F_o|^2} \right] = 0 \tag{10}$$

By substituting the value of $|F_{cT}|$ from equation (9) into equation (10) we obtain a set of equations relating the Δx_i and the observed data. If the trial model is close enough to the most probable structure, we can neglect high order terms in the series (9) because of the smallness of the Δx_i. Retaining for the present all terms through the second order, we can write equation (10) after the substitution for $|F_{cT}|$ in the form

$$\begin{aligned} 0 = \sum_u w_u \Big[(|F_o| - |F_{ct}|)(-F_k) &+ \sum_{i=1}^{m} \Delta x_i \, F_i \, F_k \\ &- \sum_{i=1}^{m} \Delta x_i \, F_{ik} \, (|F_o| - |F_{ct}|) \\ &+ \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \, \Delta x_j \, F_i \, F_{jk} \end{aligned}$$

$$+ \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \Delta x_i \, \Delta x_j \, F_k \, F_{ij}$$

$$+ \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{\ell=1}^{m} \Delta x_i \, \Delta x_j \, \Delta x_\ell \, F_{ij} \, F_{\ell k} \Big] \, .$$

If we consider only the linear terms involving derivatives with respect to x_k, we can solve for the Δx_k to obtain

$$\Delta x_k = \frac{\sum_u w_u \, (|F_o| - |F_{ct}|) \, F_k}{\sum_u w_u [F_k^2 - F_{kk} \, (|F_o| - |F_{ct}|)]}$$

This last step is definitely an approximation and essentially corresponds to neglecting all terms of the Taylor series beyond the linear one. Only the second term in the denominator arises from the second order Taylor series term. The justification for using only linear terms is made on the grounds that the Δx_k are small and that the other terms tend strongly to cancel when summed. In any case, if the model is close enough the corrections will be valid. Because of the approximations involved, an iterative procedure is used by recalculating the F_{ct} for the new parameters and determining the new correction. The new corrections are usually too large and so, to prevent oscillation, they are reduced by a constant factor before the next cycle. It is possible to include many of the other terms, but this requires much more calculation. Several cycles of the linear approximation could be computed in the time it would take to compute more accurate corrections. Convergence, if it occurs, is usually rapid enough to make the linear approximation quite satisfactory. There is good reason to think that one might get convergence from a poorer model if more of the cross derivatives were included. This is difficult, but not impossible to do using the I.B.M. 650.

The second term in the denominator is usually neglected also. This may not be a good approximation in some cases. Since this term is quite easy to include, it would probably be worthwhile to include it. The size of this correction may be judged from the ratio of one term in the denominator to F_k^2. This ratio is, if a center of symmetry is assumed,

$$1 - \frac{|F_{ct}|}{F_{ct}} \left(|F_o| - |F_{ct}|\right) \frac{\partial^2 F}{\partial x_k^2} \left(\frac{\partial F}{\partial x_k}\right)^{-2} \Bigg|_{x_k \text{ for the trial model}}$$

For the atomic position parameter of the r atom in the space group $P\bar{1}$ this ratio becomes

$$1 + \left(|F_o| - |F_{ct}|\right) \frac{|F_{ct}| \cos 2\pi(hx_r+ky_r+\ell z_r)}{F_{ct}\, f_r \exp\left[-B_r \frac{\sin^2\theta}{\lambda^2}\right] \sin^2 2\pi(hx_r+ky_r+\ell z_r)}$$

where x_r, y_r and z_r are the coordinates of the r atom in fractions of the unit cell dimensions. Because of alterations of sign of the second term, the sum of such terms will tend to cancel. For the temperature factor of the r atom using the same space group the ratio becomes

$$1 - \left(|F_o| - |F_{ct}| \right) \frac{|F_{ct}|}{F_{ct}} \frac{\sin^2\theta}{\lambda^2} \left(\frac{\partial F}{\partial B_r} \right)^{-1}$$

Again such terms tend to cancel. In the early states of refinement, however, these differences tend to be systematic in sign and will then not cancel. It would appear that the inclusion of this term, particularly for temperature factor corrections, would be advisable.

The standard deviation of the parameters so obtained may be estimated (18) from the equation $\sigma^2(x_r) = \frac{\sigma^2}{D} B_{rr}$

where $\sigma^2 = \dfrac{\sum_u w_u \left(|F_o| - |F_{ct}| \right)^2}{u - m}$

u = total number of reflections,

m = total number of parameters being varied,

B_{rr} = r'th principle minor of D,

$$D = \begin{vmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{12} & b_{22} & \cdots & b_{2m} \\ \cdot & & \cdots & \cdot \\ b_{1m} & & \cdots & b_{mm} \end{vmatrix} ,$$

$$b_{ij} = \sum_u w_u \left[F_i F_j - \delta_{ij} \left(|F_o| - |F_{ct}| \right) F_{ij} \right] .$$

If b_{rj} $(j \neq r) \ll b_{rr}$, which will be the case if the peaks are well separated in an orthogonal cell,

$$\frac{B_{rr}}{D} = \frac{1}{b_{rr}}$$

and so

$$\sigma^2(x_r) = \frac{\sum_u w_u \left(|F_o| - |F_{ct}|\right)^2}{(u-m) \sum_u w_u \left[F_r^2 - \delta_{ir}\left(|F_o| - |F_{ct}|\right) F_{ir}\right]}$$

Since the values of $\sigma^2(x_r)$ have real meaning only when the refinement is completed, the term $\delta_{ir}\ (|F_o| - |F_{ct}|)\ F_{ir}$ can be ignored as it must tend to vanish in the sum.

A very good least squares program, written by M. E. Senko and D. H. Templeton (12) is available and has been used for many of the calculations involved in the following structural investigations. A brief description of this program will be given in the next section. The purpose of this description is to place in context the modifications discussed in the L.S.II M program.

2. L.S.II program

In the Senko-Templeton L.S.II program (12), the corrections to the parameters are computed by neglecting all second order terms in the Taylor series expansion and by neglecting all first order cross terms except those between x and z for the same atom and those between the temperature factor of the first atom and the scale factor. The standard deviations are computed in a corresponding manner.

The structure factor and its derivatives are computed only for orthorhombic space groups. This subroutine can be rewritten for other space groups. In orthorhombic systems, the trigonometric part of the structure factor takes for its A part one of the forms

$$\cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z$$
$$-\cos 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \cos 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$

and for its B part one of the forms,

$$\sin 2\pi hx \cos 2\pi ky \cos 2\pi \ell z$$
$$\cos 2\pi hx \sin 2\pi ky \cos 2\pi \ell z$$
$$\cos 2\pi hx \cos 2\pi ky \sin 2\pi \ell z$$
$$-\sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$$

where $F(hk\ell) = A + iB$. The form to be used is specified by appropriate codes on each reflection card. These forms, of course, must be multiplied by multiplicity factors, temperature factor corrections, and scattering factors to form the structure factor.

3. L.S.II M program

Because of the frequent occurrence of other crystal classes, a somewhat more flexible structure factor section was desired. This flexibility can be achieved by summing an arbitrary number of the various orthorhombic forms. If, in addition, the indices can be changed and more sets of sums added to the first set the program is suitable for essentially all space groups. The modifications to the L.S.II program are designed to accomplish this flexibility.

The structure factor and derivative subroutines are modified so as to accumulate results in work cells rather than only storing them in the work cells. An added routine, just before the make up of the arguments section will zero the work cells. Thus, for any one atom, the calculations are started with zero in each work cell. The subroutine exits have been so modified that after a B part has been obtained the corresponding A part is obtained and then the program refers to address 1999 of the magnetic drum storage of the I.B.M. 650. If two or more orthorhombic type terms are desired for the same indices, the A type subroutine exits are modified so as to refer to the entrance of the next desired term. The results are automatically accumulated. The program will, in any case, finally exit at 1999. At this point, an index modification routine may be inserted, and the program is then returned to the make up of arguments routine for the calculation of the next set of terms which are also automatically summed with the previous results. This can be repeated as many times as is required. When the final structure factor and its derivatives are obtained, the modified program exits into the normal program. This requires the use of control cards which will couple the orthorhombic type routines as desired. If index modifications are required a short sub-routine must be written and inserted at 1999.

There are a few other minor modifications to the L.S.II program which expand its usefulness. For details please refer to Appendix C.

III. STRUCTURAL DETERMINATIONS

A. Structure of $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

1. Data

Preliminary X-ray diffraction photographs using the Weissenberg and precession cameras verified the assignment by J. A. A. Ketelaar (10) of the space group C_{6h}^2 - $P6_3/m$. The only systematically missing reflections were of the type (00ℓ) with $\ell = 2n + 1$. Photographs taken with long exposure times indicated that the missing (00ℓ) reflections could not have an intensity above the background level. This would indicate that the true space group is probably either C_6^6 - $P6_3$ or C_{6h}^2 - $P6_3/m$, since general positions in the space group must be occupied. The structure was refined on the basis of the centrosymmetric space group C_{6h}^2 - $P6_3/m$. The excellent final results further confirm this symmetry.

A small crystal was mounted in such a way as to record the $(h0\ell)$ reflections on a back reflection Weissenberg camera. Measurement of the positions of these reflections at large angle gives lattice constants of $a = b = 13.915 \pm 0.001$ Å and $c = 7.064 \pm 0.002$ Å. The lattice constants reported by J. A. A. Ketelaar (10) are not quite as accurate, but the above values are within his limits of error. From the density of 1.96 (10) the number of formula weights per unit cell is found to be two.

The photographs to be used for intensity measurements were obtained using an approximately cylindrical crystal 0.5 mm in length and 0.1 mm in diameter. The axis of the cylinder was the crystallographic c-axis. The crystal was coated with a thin layer of Canada balsam to prevent loss of water. Molybdenum K_{α} radiation was obtained by filtering the radiation from a molybdenum X-ray tube through zirconium foil. Data were obtained, using this K_{α} radiation, by rotating the crystal about the c-axis in a Weissenberg camera and recording each layer line so produced. A total of nine layers, including the zero layer, were recorded. Two sets of standards spots were obtained. The spots used for the standard sets were taken from the zero and third layers. By judging the intensities of a given layer against that set of standard spots which had the same size and shape, it was possible in large measure to compensate for the variations of spot shape. Several film packs, with six films per pack, were exposed for varying times for each layer so that the intensities would overlap. The film transmission factor of Eastman Kodak X-ray film for molybdenum is 0.736. Each spot was judged on each film as long as it was in the range of the standard spots. By use of the film factor, all intensities were scaled up to the first, most intense, film and averaged. The average was taken using weights related to the reproducibility of measurement in the different parts of the standard spot range.

A standard judging procedure was set up and the actual intensity judgements were made by Mrs. Jean Kestel. Mrs. Kestel was unfamiliar with this work and was quite free of any bias in judging. After a very brief instruction period she was able to do an excellent job of judging the intensities. As she did not know the transmission factor of the film, each measurement of one reflection was quite independent of the others. To save confusion, the reflections were indexed by an overlying grid of lines on tracing plastic. One set of lines was numbered and each line corresponded to reflections having a common h value. The intersecting lines were lettered and each line corresponded to reflections having a common h + k value. This procedure gives a grid with each line crossing the others with a large angle of intersection, an aid in preventing mistakes. If the grid were the regular Weissenberg net, the intersections could occur at small angles with resulting uncertainties. The actual ($hk\ell$) indices were assigned from a knowledge of the letter and number assigned to the reflection by the grid. Each reflection was judged on as many films as possible. The data were then checked, indices assigned, and weighted averages computed. This procedure worked out with complete satisfaction. Approximately 1300 reflections were judged in this manner.

The reflection intensities were corrected for Lorentz and polarization factors by means of the INCOR (19) program for the I.B.M. 650. The INCOR program also evaluates

$\sin^2\theta/\lambda^2$ and looks up the values of the atomic form factors from tables punched into cards. Atomic form factors for carbon and oxygen were obtained from the work of J. Berghuis et al. (20), that for sulfur has been computed by H. Viervol and O. Ogrim (21), and that for erbium was obtained from the work of Thomas and Umeda (22). The values of $F(hk\ell)$ so obtained are given in Appendix D.

2. Trial structure

The possible sets of equivalent positions in the space group $P6_3/m$ are given in the International Tables for X-ray crystallography (23) and are reproduced in Table 1. The coordinates are given in terms of fractions of the unit cell.

As there are only two molecules per unit cell (10), the two erbium atoms must be assigned to one of the two fold sets. The erbium scattering power is so great that if it were assigned to either set a or set b the layers for odd values of ℓ would be composed of comparatively weak reflections. As this is not the case, the erbium atoms must be assigned either to set c or to set d. These two sets differ only in the position of the origin of the unit cell, and so set c was selected.

A two dimensional electron density projection using the (hk0) data and the signs of the erbium structure factor contribution was computed by the use of the T.D.F. 40-80 program for the I.B.M. 650. Because of the sixfold symmetry,

Table 1. Equivalent positions for space group $P6_3/m$

Wyckoff notation and point symmetry		Co-ordinates of equivalent positions			Conditions limiting possible reflections
i	1	$x,y,z;$	$\bar{y},x-y,z;$	$y-x,\bar{x},z;$	$(00\ell):\ell=2n$
		$\bar{x},\bar{y},\bar{z};$	$y,y-x,\bar{z};$	$x-y,x,\bar{z};$	
		$\bar{x},\bar{y},\frac{1}{2}+z;$	$y,y-x,\frac{1}{2}+z;$	$x-y,x,\frac{1}{2}+z;$	
		$x,y,\frac{1}{2}-z;$	$\bar{y},x-y,\frac{1}{2}-z;$	$y-x,\bar{x},\frac{1}{2}-z.$	
h	m	$x,y,\frac{1}{4};$	$\bar{y},x-y,\frac{1}{4};$	$y-x,\bar{x},\frac{1}{4};$	
		$\bar{x},\bar{y},3/4;$	$y,y-x,3/4;$	$x-y,x,3/4.$	$(00\ell):\ell=2n$
g	$\bar{1}$	$\frac{1}{2},0,0;$	$0,\frac{1}{2},0;$	$\frac{1}{2},\frac{1}{2},0;$	$(hk\ell):\ell=2n$
		$\frac{1}{2},0,\frac{1}{2};$	$0,\frac{1}{2},\frac{1}{2};$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
f	3	$1/3,2/3,z;$	$2/3,1/3,\bar{z};$		$(hk\ell)$: if $h-k=3n$ then $\ell=2n$
		$2/3,1/3,1/2+z;$	$1/3,2/3,1/2-z.$		
e	3	$0,0,z;$	$0,0,\bar{z};$		$(hk\ell):\ell=2n$
		$0,0,\frac{1}{2}+z;$	$0,0,\frac{1}{2}-z.$		
d	$\bar{6}$	$2/3,1/3,1/4;$	$1/3,2/3,3/4.$		$(hk\ell)$: if $h-k=3n$ then $\ell=2n$
c	$\bar{6}$	$1/3,2/3,1/4;$	$2/3,1/3,3/4.$		
b	$\bar{3}$	$0,0,0;$	$0,0,1/2.$		$(hk\ell):\ell=2n$
a	$\bar{6}$	$0,0,1/4;$	$0,0,3/4.$		

for each reflection (hk0) there are five other equivalent reflections ($\bar{k}\bar{i}0$), (ih0), ($\bar{h}\bar{k}0$), (ki0), and ($\bar{i}\bar{h}0$) where $i = \bar{h} + \bar{k}$. Only the monoclinic symmetry could be used in reducing the number of required coefficients for the Fourier summation. Consequently the reflections (hk0), (ki0) and ($\bar{i}\bar{h}0$) must be separately included. The atoms in the unit cell were remarkably well resolved in this projection, and rough x and y parameters for all of the atoms except for the carbons and the hydrogens were obtained. There were indications of possible carbon positions, but the interpretation of them was somewhat ambiguous. The rough parameters so obtained are given in Table 2.

The z-parameters can not be obtained directly from the electron density projection. However, from a knowledge of reasonable atomic radii, it is possible to assign either one of two sets of z-parameters. These two sets are given in Table 2 where either the upper set or the lower set of values may be used. The sixfold water molecules and the sulfur atoms cannot have the same z-parameter as this would place the water and a sixfold sulfate oxygen too close together. From a knowledge of the sulfate ion structure, the z-parameter, relative to the sulfur, can be deduced. The further assumption that the twelvefold water molecules are hydrating the metal ion allows an estimate of their z-parameters to be made. There was no very convincing way to

Table 2. Rough parameters from electron density projection

Number of positions and point symmetry		Atom	Co-ordinates x	y	z
2	$\bar{6}$	Erbium	0.333	0.666	0.250
6	m	Sulfur	0.319	0.371	0.250 0.750
6	m	Sulfate Oxygen	0.247	0.418	0.250 0.750
6	m	Sulfate Oxygen	0.224	0.242	0.250 0.750
12	1	Sulfate Oxygen	0.381	0.390	0.069 0.569
6	m	Water Oxygen	0.337	0.490	0.750 0.250
12	1	Water Oxygen	0.215	0.550	0.562

distinguish the two models from the information given by the (hk0) data and atomic radii.

3. Refinement of the trial structure

The trigonometric part of the structure factor expression for one general set of atoms is given for $\ell = 2n$ by

$$4 \cos 2\pi\ell z \left[\cos 2\pi(hx+ky) + \cos 2\pi(ky+iy) + \cos 2\pi(ix+hy)\right]$$

and for $\ell = 2n + 1$ by

$$-4 \sin 2\pi \ell z \left[\sin 2\pi(hx+ky) + \sin 2\pi(kx+iy) + \sin 2\pi(ix+hy)\right],$$

where $i = \bar{h} + \bar{k}$. This form is not suitable for computation by the L.S.II M program. By expansion, the above forms can be written as,

for $\ell = 2n$,

$$4 \left[\cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z - \sin 2\pi hx \sin 2\pi ky \cos 2\pi \ell z + \cos 2\pi kx \cos 2\pi iy \cos 2\pi \ell z - \sin 2\pi ky \sin 2\pi iy \cos 2\pi \ell z + \cos 2\pi ix \cos 2\pi hy \cos 2\pi \ell z - \sin 2\pi ix \sin 2\pi hy \cos 2\pi \ell z\right]$$

and for $\ell = 2n + 1$,

$$-4 \left[\sin 2\pi hx \cos 2\pi ky \sin 2\pi \ell z + \cos 2\pi hx \sin 2\pi ky \sin 2\pi \ell z + \sin 2\pi kx \cos 2\pi iy \sin 2\pi \ell z + \cos 2\pi kx \sin 2\pi iy \sin 2\pi \ell z + \sin 2\pi ix \cos 2\pi hy \sin 2\pi \ell z + \cos 2\pi ix \sin 2\pi hy \sin 2\pi \ell z\right].$$

By the use of the L.S.II M program, this form can be evaluated and the proper derivatives can be obtained. For each pass through the structure factor and derivative section, one pair of the six terms is evaluated and their derivatives are obtained. The indices are then altered and the next pair is evaluated and summed with the first pair. A second index modification follows and then the third term is computed and summed. The indices are then restored to their original values and the regular L.S.II program is entered again. The work cells used above are reset just before the first entrance to the structure factor routine for each atom. In this program, the multiplicity factor used is one for the general 12 fold set and proportionately less for special sets. This involves adding a factor of 1/6 to those available in the program.

A few cycles of refinement of the (hkl) data using the erbium and sulfur parameters of each of the two possible trial models clearly indicated that the correct structure is the one assigning a z-parameter of 0.750 to the sulfur set of atoms. This then forces the choice of the remaining z-parameters to be the lower ones of the pairs given in Table 2. It should be noted that large corrections to the erbium parameters were indicated. This is, of course, nonsense. The reason for this is that the positional derivatives of the erbium positions vanish identically. Because of the 1/3 and 2/3 in the parameters and because of the method used to obtain the sines and cosines, enough error is introduced to produce a correction which is the ratio of two error terms. This results in erratic and meaningless corrections to the parameters of the erbium atoms. This can be taken care of by simply resetting the erbium parameters before each cycle.

The refinement of the trial model obtained above was carried out by least squares cycles using the (hk0) data. The z-parameters were, of course, not refined by this procedure. A constant weighting factor was used and values of

$R_1 = 0.1198$ and of $R_2 = 0.0193$ were obtained. R_1 and R_2 are defined by

$$R_1 = \frac{\sum_u (|F_o| - |F_{ct}|)}{\sum_u |F_o|}$$

$$R_2 = \frac{\sum_u (|F_o| - |F_{ct}|)^2}{\sum_u |F_o|^2} \quad ,$$

and are a measure of the agreement between the model and the data. Because of the errors in measuring the data an agreement factor of $R_1 \sim 0.1$ implies very good agreement. The R factor alone, however, is not enough to justify a model since a few important reflections may be matched very poorly. This would indicate that changes must be made in the model. Such was not the case here.

A few signs of the F(hk0) were changed by the inclusion of the other atoms and so another electron density projection was obtained. The carbon positions were still ambiguous, but it was possible, from packing considerations, to assign approximate parameters. These parameters were $x = 0.186$, $y = 0.031$ and $z = 0.750$ for one sixfold set of carbons and $x = 0.287$, $y = 0.181$ and $z = 0.750$ for the other sixfold set of carbon atoms. The inclusion of these carbon parameters lead to a further refinement of the model by least squares. The agreement factors thus obtained were $R_1 = 0.0884$ and

Table 3. Results of two dimensional least squares refinement of $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	(Z)	σ_x	σ_y
Er	01	1.37	0.3333	0.6666	0.2500	-	-
S	02	2.34	0.3205	0.3725	0.7500	0.0008	0.0008
$O(SO_4)$	03	2.83	0.2489	0.4211	0.7500	0.0022	0.0022
$O(SO_4)$	04	2.55	0.2259	0.2357	0.7500	0.0022	0.0021
$O(SO_4)$	05	3.68	0.3828	0.3960	0.569	0.0013	0.0013
$O(H_2O)$	06	3.29	0.3494	0.4927	0.2500	0.0024	0.0025
$O(H_2O)$	07	2.45	0.2133	0.5463	0.562	0.0011	0.0011
$C(CH_3)$	08	3.09	0.1767	0.0524	0.7500	0.0034	0.0034
$C(CH_2)$	09	3.12	0.2744	0.1671	0.7500	0.0034	0.0034

R_2 = 0.0097 which indicate remarkable agreement with the data. The resulting parameters, with their standard deviations are given in Table 3.

The set number used in Table 3 is merely an identification number used to keep the cards and calculations consistent. B is the temperature factor.

It is interesting to note the manner in which the scale factors, the temperature factors, and the positional parameters converged using the least squares method. The starting model was most accurate with respect to positional parameters. The initial scale factors were approximate but crude. The initial temperature factors were just guesses but were approximately correct. The positional parameters moved very little in the first stages of refinement while the scale factor was refining. The temperature factors invariably increased during this period. Then in the middle part of the refinement, after the scale factor settled down the parameters would adjust. The temperature factors would remain steady or continue to increase. Then in the last stages, the temperature factors would drop sharply to their final values. This seems to be a quite general behavior as a similar behavior has been noted in essentially all of the least squares calculations for this and other structures. From this behavior, the conclusion that faster convergence for the temperature factor would substantially speed up the overall convergence would appear to be valid. The behavior of the temperature factor indicates that the approximations used in computing temperature factor corrections are not very satisfactory when the error in the temperature factor is not very small. Because of the lack of oscillation in the temperature factor, the damping factor for the corrections is satisfactory. The linear diagonal term arising from the second order term of the Taylor series expansion is not used in the L.S.II program. The form of this term is such as possibly to account for the temperature factor behavior. It would be interesting to include this term but this has not been done as yet.

A least squares refinement using all of the data, about 1600 reflections including unobserved intensities, was carried out. The temperature factors and parameters from the two dimensional refinement cycles were used for the first three dimensional cycle of refinement. Approximate scale factors for each layer were obtained by taking a small number of reflections from each layer and refining crude guesses while holding all other parameters fixed. This was a very fast operation and it saves possibly several complete cycles with the bulk of the data. These scale factors were then used for the first three dimensional cycle. Each three dimensional cycle required approximately nine hours time on the I.B.M. 650. Five such cycles were computed using constant weighting factors and the results are shown in Table 4 and Table 5. The agreement factors for the complete data are $R_1 = 0.1016$ and $R_2 = 0.0203$ and are quite satisfactory.

The observed data and the calculated structure factors based on the above structure are given in Appendix D.

The signs of F(hk0) obtained from the above structure were used to recalculate the electron density projection onto the (001) plane. The values of $F_{obs}(010)$, $F_{obs}(020)$, $F_{obs}(110)$, $F_{obs}(120)$ and $F_{obs}(210)$ could not be obtained from the films since they occurred at too small a reflection angle. Since these reflections are very insensitive to the

Table 4. Scale factors and R values for $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Layer (ℓ)	Scale factor	R_2	Layer (ℓ)	Scale factor	R_2
0	9.746	0.0109	5	10.394	0.0303
1	8.255	0.0238	6	11.876	0.0395
2	9.146	0.0122	7	13.564	0.0321
3	8.048	0.0197	8	13.92	0.0391
4	9.143	0.0168	all	-	0.0203

Table 5. Parameters for $Er(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	Z	σ_x	σ_y	σ_z
Er	01	1.27	.3333	.6666	.2500	-	-	-
S	02	2.02	.3191	.3720	.7500	.0003	.0003	-
O	03	2.83	.2489	.4216	.7500	.0012	.0012	-
O	04	2.80	.2289	.2425	.7500	.0012	.0012	-
O	05	3.43	.3826	.3948	.5780	.0009	.0009	.0019
O	06	2.67	.3509	.4947	.2500	.0011	.0011	-
O	07	2.72	.2138	.5458	.4868	.0008	.0008	.0017
C	08	3.95	.1772	.0523	.7500	.0020	.0020	-
C	09	4.01	.2727	.1693	.7500	.0020	.0020	-

parameters, the calculated values of these reflections were used in the electron density projection. The F(000) term has been omitted and the electron density function was computed with an arbitrary scaling factor. The resulting projection is shown in Figure 1. It can be seen that good resolution is obtained and even the carbon peaks are clearly defined. This resolution, in the presence of the heavy erbium atoms, is much better than one previously would have thought possible.

B. Structure of $Y(C_2H_5SO_4)_3 \cdot 9H_2O$

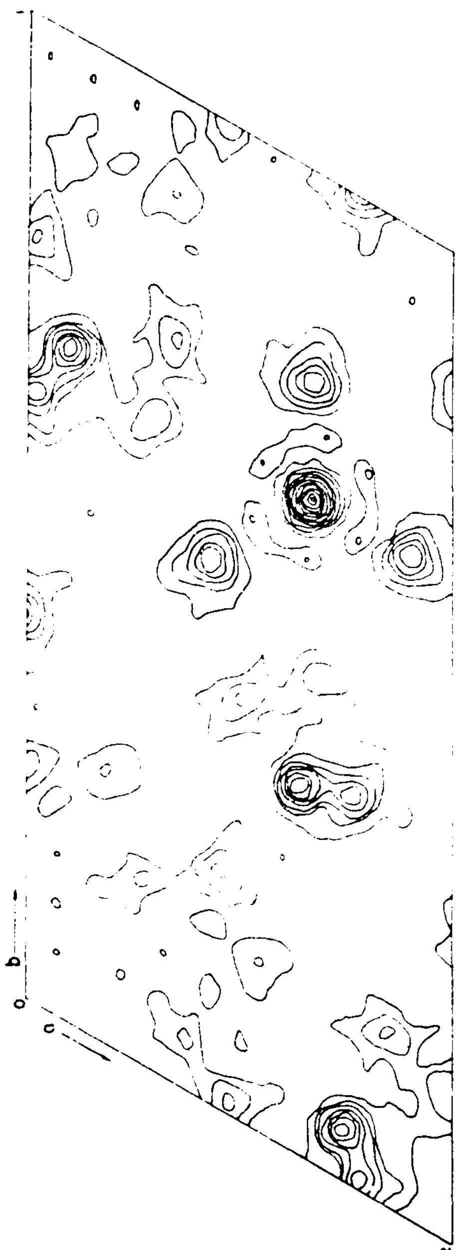
1. Data

The preliminary data again, and for the same reasons, indicated that the assignment of the C^2_{6h} - $P6_3/m$ space group to this compound by J. A. A. Ketelaar (10) was correct. A precision determination of the lattice constants by a back reflection technique gave the values a = b = 13.9245 0.001 Å and c = 7.057 0.002 Å. This indicated that the $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ was isomorphous to the $Er(C_2H_5SO_4)_3 \cdot 9H_2O$ crystal.

Because of the fluorescence of yttrium in molybdenum K_α radiation, copper K_α radiation was used to obtain the intensity data. It was possible to obtain data using the Weissenberg camera for only five layers including the zero layer. Approximately 600 reflections were measured. The

Figure 1. The projection of the electron density of erbium ethylsulfate onto the (001) plane

The value of F(000) was omitted in this calculation and an arbitrary scaling factor was used. The contours are therefore in arbitrary units. The contours about the erbium atom are spaced at four times the value of the other contours.


o
b
c
a

judging procedure was the same as that used in the case of the erbium compound. The measured intensities were then corrected for the Lorentz and polarization factors by use of the INCOR program (19).

The intensities indicated that the only possible difference between the yttrium and erbium structures was one of small parameter shifts. Consequently, the parameters of the $Er(C_2H_5SO_4)_3 \cdot 9H_2O$ structure were used as the trial model for the yttrium compound. A projection of the electron density onto the (001) plane gave essentially the same results as for the erbium compound.

2. Refinement of the trial structure

In order to reduce the required number of three dimensional refinement cycles, the x and y parameters were refined using the (hk0) data only. Four cycles of least squares refinement using constant weighting factors were computed. The resulting parameters are given in Table 6. The agreement factors attained are $R_1 = 0.0913$ and $R_2 = 0.0125$.

There is reason to believe that the true weighting factors which should be used in a least squares refinement are not constant. The true weighting factors should be inversely proportional to the square of the probable error of the corresponding observed structure factor magnitude (18). Mr. Donald E. Williams (16) studied the measurement errors and concluded that it would be reasonable to assume that the

Table 6. Results of two dimensional least squares refinement of $Y(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	(Z)	σ_x	σ_y
Y	01	2.49	.3333	.6666	.2500	-	-
S	02	2.25	.3176	.3713	.7500	.0004	.0004
O	03	2.74	.2451	.4121	.7500	.0009	.0009
O	04	3.69	.2355	.2467	.7500	.0012	.0012
O	05	3.99	.3836	.3948	.5780	.0006	.0006
O	06	4.82	.3463	.4911	.2500	.0014	.0014
O	07	2.89	.2127	.5446	.4868	.0006	.0005
C	08	7.34	.1726	.0442	.7500	.0026	.0033
C	09	3.59	.2734	.1657	.7500	.0019	.0018

probable error in the observed structure factor magnitudes is given by the formulae

$$\Delta F_o = \frac{c}{200} F_o \quad \text{for} \quad I_o \geq 16\ I_m,$$

and

$$\Delta F_o = \frac{kF_m^2}{2\ F_o} \quad \text{for} \quad I_o < 16\ I_m,$$

where c = percentage error in observed intensities I_o,

kI_m = absolute error in I_o

I_m = background intensity

F_m = value of F corresponding to I_m.

To a first approximation, F_m^2 is a constant and so, in the second case above, ΔF_o is inversely proportional to F_o. The corresponding weighting factor expressions were programmed and inserted into the L.S.II M program. Any reference to variable weighting factors in the following discussion will mean the weighting factors based upon the above errors. It should be mentioned that, when variable weighting factors are used, a third R value, R_3, is obtained from the L.S.II and the L.S.II M programs. R_3 is defined by

$$R_3 = \frac{\sum_u w_u(|F_o| - |F_{ct}|)^2}{\sum_u w_u |F_o|^2}$$

and is an especially sensitive measure of agreement.

Least squares refinements using all of the data were carried out using both constant and variable weighting factors. Five cycles using constant weights were followed by two cycles using variable weights. Because of the previous constant weight refinement, the variable weight refinement converged in the two cycles. This does not indicate faster convergence with variable weights. The results of this refinement procedure are given in Table 7 and Table 8. The upper values in each table are the results of constant

Table 7. Scale factors and R values for $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ for refinement with constant (upper values) and variable (lower values) weighting factors

Layer	0	1	2	3	4	All
Scale Factor	2.024 1.997	2.143 2.175	2.325 2.295	1.838 1.751	1.661 2.153	- -
R_3	0.0048 0.0052	0.0041 0.0035	0.0048 0.0048	0.0076 0.0055	0.0119 0.0092	0.00607 0.00537
R_2	0.0089 -	0.0082 -	0.0099 -	0.0097 -	0.0245 -	0.0102 0.0117
R_1	- -	- -	- -	- -	- -	0.0808 0.0881

weighting factors and the lower values are the results for variable weighting factors. The R_3 values for constant weights were obtained from the next, variable weight cycle.

It can be seen that the use of variable weighting factors did not affect the R factors very much but that there was some change in scale factors. The large change in the scale factor for the fourth layer is probably due to the preponderance of weak reflections in that layer.

The temperature factors for the light elements are somewhat dependent upon the weighting factors used. This should sound a note of warning about the use of anisotropic temperature factors. Anisotropic factors should be even more

Table 8. Parameters for $Y(C_2H_5SO_4)_3 \cdot 9H_2O$ for constant (upper values) and variable (lower values) weighting factors

Atom	Set number	B	X	Y	Z	σ_x	σ_y	σ_z
Y	01	2.47 2.65	.3333 .3333	.6666 .6666	.2500 .2500	- -	- -	- -
S	02	2.58 2.34	.3187 .3195	.3715 .3715	.7500 .7500	.0003 .0005	.0003 .0005	- -
O	03	3.85 4.29	.2485 .2482	.4205 .4188	.7500 .7500	.0009 .0013	.0009 .0013	- -
O	04	3.97 4.47	.2298 .2305	.2443 .2446	.7500 .7500	.0009 .0014	.0009 .0014	- -
O	05	3.95 4.28	.3837 .3833	.3947 .3940	.5763 .5759	.0006 .0008	.0006 .0009	.0014 .0015
O	06	3.01 3.11	.3525 .3524	.4936 .4920	.2500 .2500	.0008 .0011	.0008 .0013	- -
O	07	3.17 3.26	.2122 .2129	.5452 .5462	.4854 .4873	.0005 .0008	.0005 .0008	.0014 .0021
C	08	5.76 6.71	.1793 .1815	.0515 .0526	.7500 .7500	.0017 .0023	.0017 .0023	- -
C	09	4.63 5.74	.2751 .2755	.1650 .1655	.7500 .7500	.0015 .0025	.0015 .0025	- -

sensitive to systematic errors in the data. The use of such factors should be valid only if all systematic errors in the data and calculations are properly accounted for. This is obviously not true for these data. However, the differences in the temperature factors above should give a good measure of the accuracy to be expected in the isotropic temperature factors.

Fortunately, it appears that the weighting factors have little effect on the positional parameters. The largest difference, aside from the carbon parameters, amounts to only 0.02 Å in the parameter. One carbon parameter changed by 0.03 Å. These changes are of the same order as the standard deviations in the parameters.

The observed data and the calculated structure factors are given in Appendix D.

C. Structure of $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$

1. Data

Preliminary photographs verified that the praseodymium compound is isomorphous with the erbium and yttrium compounds. Because there was interest in the symmetry of the water molecules about the rare earth ion and because small differences from the erbium compound might not affect the intensities very much, partial data was obtained and analyzed. Precision cell constants were not measured. The cell constants determined by J. A. A. Ketelaar (10) were used in this investigation. The cell constants are a = b = 14.035 Å and c = 7.104 Å.

The (hk0) data were obtained using a Weissenberg camera and molybdenum radiation. The intensities were judged in the same manner as for the erbium and yttrium compounds. The intensities were corrected for Lorentz and polarization factors by the INCOR (19) program. Comparison of these intensities with the (hk0) intensities of erbium indicated a very close correlation. Consequently, the structure of the erbium compound should be a satisfactory trial model for the refinement of this structure. The data so obtained is given in Appendix D.

2. Refinement of the trial structure

Four cycles of L.S.II M refinement were enough to give convergence from the trial model. Constant weighting factors were used. The agreement factors were R_1 = 0.0951 and R_2 = 0.0157. The parameters obtained are given in Table 9.

The Y parameter for set O5 is chosen so as to give a consistent S - O distance and is 0.5770. The Y parameter for set O7 is estimated, from the increase in the size of the rare earth ion, to be 0.4947.

The high temperature factor, B, for set O5 is probably due to insufficient resolution of this set from the set of sulfur atoms. The shifts in the parameters are small enough

Table 9. Parameters of $Pr(C_2H_5SO_4)_3 \cdot 9H_2O$

Atom	Set number	B	X	Y	σ_x	σ_y
Pr	01	1.03	.3333	.6666	-	-
S	02	1.81	.3178	.3710	.0008	.0008
O	03	2.79	.2476	.4207	.0024	.0024
O	04	2.92	.2292	.2422	.0025	.0025
O	05	3.67	.3819	.3958	.0014	.0014
O	06	3.03	.3570	.4908	.0026	.0025
O	07	2.90	.2081	.5418	.0012	.0013
C	08	3.60	.1786	.0566	.0041	.0040
C	09	4.13	.2763	.1748	.0044	.0044

to indicate that there is little difference between the praseodymium and erbium compounds except for the size of the rare earth ion.

D. Discussion of Structures

1. Coordination of the rare earth ion

The structures of the erbium, yttrium and praseodymium ethylsulfates are essentially identical within experimental error, the sole difference being one of ionic size. The general features of this structure are shown in Figure 2.

The rare earth ion is surrounded by nine water oxygens with the symmetry C_{3h}. Six water oxygens are placed above and below the rare earth ion at the six corners of a triangular prism. The remaining three water oxygens are placed out from the three vertical faces of the prism in the same plane as the rare earth ion. These three water oxygens are farther away from the rare earth ion than are the six above and below the rare earth ion. The metal to water oxygen distances are given in Table 10. These distances were calculated by the use of the distance program (25) for the I.B.M. 650. The symmetry of this arrangement could be D_{3h} but there is a slight rotation of the water oxygens, in the plane of the rare earth ion, with respect to the six water oxygens out of the plane. A rotation of the water oxygens in the plane of 4°23', 5°5', and 6°25' for the erbium, yttrium and praseodymium compounds respectively would restore the D_{3h} symmetry. The possible positions of the hydrogen atoms will be discussed in a latter section.

The ethylsulfate oxygens are arranged about the rare earth ion with C_{3h} symmetry as shown in Figure 2. There are a total of 18 ethylsulfate oxygens as next nearest neighbors about the rare earth ion. The distances from the rare earth ion are given in Table 10. The ethyl groups are packed closely about origin of the unit cell. This packing about

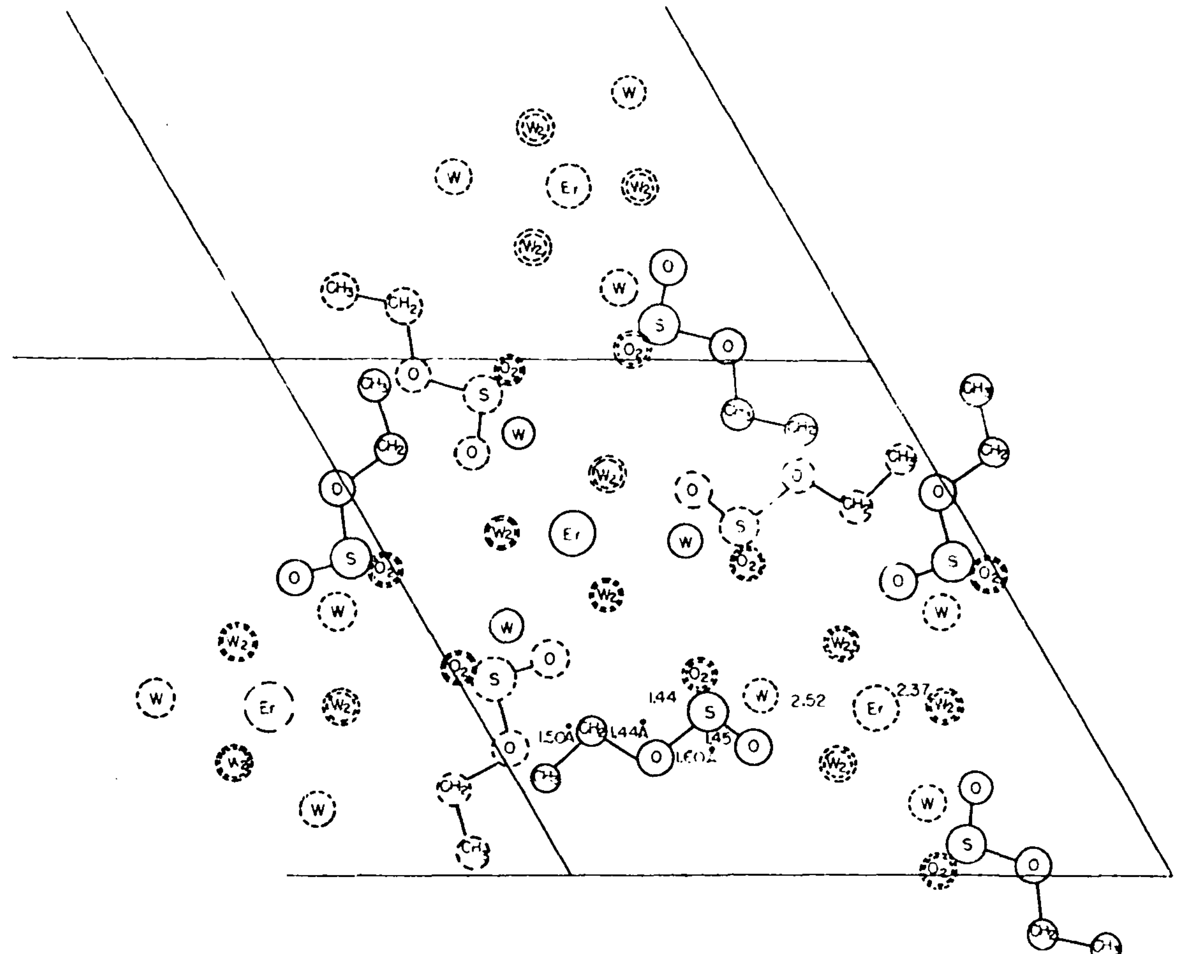


Figure 2. Packing diagram of erbium ethylsulfate

The solid circles represent atoms in the plane z = 1/4.

Table 10. Distances from the rare earth ion in Å

Atom	Set number	Quantity	Distance from Er	Distance from Y	Distance from Pr
$O(H_2O)$	06	3	2.52	2.55	2.65
$O(H_2O)$	07	6	2.37	2.37	2.47[a]
$O(-SO_4)$	03	6	4.63	4.64	4.65
$O(-SO_4)$	05	6	4.77	4.77	4.77[a]
		6	4.61	4.60	4.66[a]
$S(-SO_4)$	02	3	5.13	5.13	5.18
		6	5.33	5.34	5.36
$O(C_2H_5O-)$	04	3	5.56	5.57	5.61

[a]The calculation of these distances requires Y parameters which have been estimated from the structure of the ethylsulfate ion and from the increase in the radius of the rare earth ion.

the 6_3 axis at the origin leads to infinite cylinders of hydrocarbon material at the origin of the unit cell.

The hydrogens attached to the carbon atoms can be placed so as to preserve the C_{3h} symmetry. This requires that one of the methyl hydrogens lies in the mirror plane. The packing, with such an arrangement, is quite reasonable. There is no reason to suppose that the hydrogens violate the C_{3h} symmetry.

2. The ethylsulfate ion structure

The structure of the ethylsulfate ion has been determined during a structural investigation of potassium ethylsulfate by J. A. J. Jarvis (24) using three dimensional Fourier techniques. The distances within the ethylsulfate group are shown in Table 11. The distances for the potassium compound are also given.

Table 11. Ethylsulfate ion distances in Å

From set	To set	Distance Er	Y	Pr	K
02-S	03-0	1.45	1.45	1.46	1.49
02-S	05-0	1.44	1.46	1.45	1.44
02-S	05-0	1.44	1.46	1.45	1.45
02-S	04-0	1.60	1.57	1.60	1.60
04-0	09-C	1.44	1.52	1.40	1.44
09-C	08-C	1.50	1.47	1.54	1.51
04-0	05-0	2.45	2.45	2.47	2.46
04-0	05-0	2.45	2.45	2.47	2.44
04-0	05-0	2.37	2.33	2.39	2.41
03-0	05-0	2.40	2.42	2.41	2.43
03-0	05-0	2.40	2.42	2.41	2.30
05-0	05-0	2.43	2.45	2.44	2.36

Considering the comparatively large atomic numbers of Er and Y, the agreement with the potassium ethylsulfate results is remarkable. The spread in the equivalent S-O distances is only 0.01 Å for the heavy metal compounds. The O-C-C distances are in good agreement, although it would appear that the O9-C set for yttrium ethylsulfate has not refined as well as in the other cases. The temperature factor for this carbon is a little smaller than for the others. The differences in position are small enough to be explained by the combination of an error in the position of the O4-O set of approximately 0.03 Å with an error in the opposite direction of 0.05 Å in the position of the O9-C set. This is about the same size as the standard deviation in the positions. It should be noted, however, that with this one exception the bond lengths are self consistent with an accuracy much better than would be required by the standard deviations.

3. The position of hydrogen bonds

The actual positions of the hydrogen atoms has not, of course, been determined. The positions of hydrogen bonds can be deduced in some cases from a knowledge of the interatomic distances of the atoms which could be attached to a hydrogen. These distances are given in Table 12.

The interpretation of these distances in terms of hydrogen bonds is obviously not unambiguous. However, if there

Table 12. Oxygen-oxygen distances

From water oxygen	To atom	Set number	Number of distances	Distance Er	Y	Pr
06	Sulfate Oxygen	05	$\underline{2}$[a]	2.85	2.83	2.77[b]
	Water Oxygen	07	2	2.88	2.91	3.07[b]
	Water Oxygen	07	2	2.68	2.68	2.76[b]
07	Sulfate Oxygen	03	$\underline{1}$[a]	2.74	2.76	2.76[b]
	Sulfate Oxygen	05	1[a]	2.85	2.81	2.83[b]
	Water Oxygen	06	1	2.88	2.91	3.07[b]
	Water Oxygen	06	1	2.68	2.68	2.76[b]
	Water Oxygen	07	2	2.89	2.92	3.04[b]

[a]Underlined atoms are thought to be hydrogen bonded.

[b]These values are obtained from estimated parameters.

were hydrogen bonding between the water molecules (sets 06 and 07) it would place the corresponding protons comparatively close to the metal ion and would orient the water dipole in opposition to the strong electric field between the metal ion and the sulfate oxygens. Hydrogen bonding between the waters and the sulfate oxygens would place the protons much closer to the negative oxygens and would align the water dipoles with the electric field. The second possibility would seem to be more reasonable provided the oxygen positions produced the proper oxygen to oxygen distances and the resulting angles were reasonable. It can be seen in Table 12 that the required sulfate oxygen positions are present. The angle formed by the two set O5 oxygens with set O6 water oxygen of 107°39' is quite reasonable. The hydrogen bond distance of 2.85 is also reasonable. Hydrogen bonding in this manner could also explain the loss of D_{2h} symmetry of the water polyhedron and the longer water to metal ion distance for the set O6 oxygens. The hydrogen bonds are slightly long. This would indicate that the set O6 oxygens are balancing between the metal ion attraction and the hydrogen bond contraction. This would tend to rotate the O6 set with respect to the O7 set. This rotation would also tend to align the water dipole even more in the direction of the field. It is this rotation that is responsible for destroying the D_{3h} symmetry of the oxygen polyhedron about the metal ion.

The set O7 water oxygens can form hydrogen bonds to the set O3 and set O5 sulfate oxygens. The bonds are of unequal length, 2.74 Å and 2.85 Å, and the H-O-H angle is 94°37'. The water dipole is closely aligned with the electric field.

This hydrogen bond structure should, consequently, give the lowest energy.

It should be noted that any reasonable placement of hydrogen bonds must violate D_{3h} symmetry and produce C_{3h} symmetry.

4. The Jahn-Teller effect

As was expected from the work of J. H. VanVleck (8)(9), no Jahn-Teller distortion could be detected in the praseodymium salt. The distortions produced must be less than the experimental errors in the structure determination. Because of the excellent refinement of the (hk0) data, the threefold symmetry must be very closely obeyed.

It should be noted that the Jahn-Teller effect is not to be expected in the yttrium and erbium salts because of the occurrence of Kramers degeneracy. This is the only type of degeneracy present and no electric field can split the Kramers degeneracy. Distortions in such a case do not necessarily lead to lower energy for the molecule. An interesting derivation of Kramers degeneracy is given by J. M. Jauch (26) which clearly shows Kramers degeneracy to be independent of the field.

IV. SUMMARY

A. Computing Methods

A discussion of the various methods of evaluation of Fourier series was given. The use of the Fourier series in obtaining trial structures and in refining trial structures is discussed. These two uses require, for optimum results, different approaches. The T.D.F. 40-80 program for the I.B.M. 650 was written to satisfy the first of these needs and the T.D.F. 80 block program was written to satisfy the second of these needs.

A discussion of the least squares method as applied to refinement of crystal structures is given. A modification of the Senko-Templeton L.S.II program that will permit the use of more complex symmetry relationships in computing structure factors and in refining crystal structures has been made.

B. Structure Determination

The structures of erbium and yttrium ethylsulfate nonahydrate have been determined and refined by a three dimensional least squares method. The refinement produced R_1 values of 0.1016 for the erbium compound and of 0.0808 for the yttrium compounds for the three dimensional data. The structure of the praseodymium compound was determined by a two dimensional refinement using a least squares method. The R_1 value for these data was 0.0951. The two Z parameters were not refined.

The structures of the rare earth ethylsulfates studied are isomorphous. The symmetry about the metal ion is C_{3h}. The water molecules are arranged about the metal ion in a polyhedron of C_{3h} symmetry. The symmetry of this polyhedron is approximately D_{3h}.

The possible positions of hydrogen bonds are also discussed.

V. BIBLIOGRAPHY

1. Sayer, E. V. and Freed, S. J. Chem. Phys. 24 1213 (1956).

2. Bleaney, B., Scovil, H. E. D., and Trenam, R. S. T. Proc. Roy. Soc. (London) 223A 15 (1954).

3. Bozorth, R. M. Bell Telephone Laboratories. Private Communication (1957).

4. Spedding, F. H. and Co-workers Ames Laboratory of the Atomic Energy Commission. Private Communication (1958).

5. Jahn, H. A. and Teller, E. Proc. Roy. Soc. (London) 161 220 (1937).

6. Jahn, H. A. Proc. Roy. Soc. (London) 164 117 (1937).

7. Kramers, H. A. Proc. Acad. Sci. Amst. 33 959 (1930).

8. VanVleck, J. H. J. Chem. Phys. 7 6 (1939).

9. VanVleck, J. H. J. Chem. Phys. 7 72 (1939).

10. Ketelaar, J. A. A. Physica 4 619 (1937).

11. International Business Machines Corporation. 650 Magnetic Drum Data-Processing Machine Manual of Operation. Rev. ed. The Corp. (1955).

12. Senko, M. E. and Templeton, D. H. University of California. Private Communication (1957).

13. Lipson, H. and Cochran, W. The Determination of Crystal Structures, Chapter 1. in Bragg, L., ed. The Crystalline State, Volume 3. London, G. Bell and Sons, Ltd. (1953).

14. Lipson, H. and Cochran, W. The Determination of Crystal Structures, Chapter 1. in Bragg, L., ed. The Crystalline State, Volume 3. London, G. Bell and Sons, Ltd. (1953).

15. James, R. W. The Optical Principles of the Diffraction of X-Rays, Chapter 2. in Bragg, L., ed. The Crystalline State, Volume 2. London, G. Bell and Sons, Ltd. (1954).

16. Williams, D. Ames Laboratory of the Atomic Energy Commission. Private Communication (1957).

17. Hughes, E. W. J. Am. Chem. Soc. 63 1737 (1941).

18. Whittaker, E. T. and Robinson, G. The Calculus of Observations, Chapter 8. London, Blackie and Son (1941).

19. Templeton, D. H. University of California. Private Communication (1957).

20. Berghuis, J., Haanappel, I. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendaal, A. L. Acta Cryst. 8 478 (1955).

21. Viervol, H. and Ogrim, O. Acta Cryst. 2 277 (1949).

22. Thomas, L. H. and Umeda, K. J. Chem. Phys. 26 293 (1957).

23. Henry, N. F. M. and Lonsdale, K. International Tables for X-Ray Crystallography, Volume 1. Birmingham, England. The Kynoch Press (1952).

24. Jarvis, J. A. J. Acta Cryst. 6 327 (1953).

25. Templeton, D. H. University of California. Private Communication (1957).

26. Jauch, J. M. U. S. Atomic Energy Commission Report, ORNL 813 (Oak Ridge National Laboratory Report). September 15, 1950. (Office of Technical Services, Washington 25, D. C.)

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VII. APPENDIX A: T.D.F. 80 B PROGRAM

A. Fourier Series Evaluation for a 4x4x4 Point Block

1. Mathematical method

This program carries out the Fourier synthesis

$$\rho(x,y,z) = \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{\ell=0}^{\infty} |F(hk\ell)| \cos 2\pi(hx+ky+\ell z\pm\alpha)$$

in three dimensions within the unit cell on lattice points formed by subdivision of the unit cell at intervals of 1/80th. The series is evaluated for an arbitrary 4x4x4 point block. $F(hk\ell)$ is the structure factor and α is the phase angle, expressed as an integral multiple of 1/80th. The quantity actually entered into the 650 is α' where $\alpha' = n/80$ (4000) and $n = 0,1,2,\ldots,79$. The first four sections of the program locate and store the necessary cosines from three cosine decks located at optimum intervals on the drum. The breakdown of the program into sections is indicated in the flow diagram, Figure 3. Each cosine deck occupies two full lines (80 storages) across the drum, with the first line running from zero to $39/40\pi$ and the second from π to $79/40\pi$. Cosines are located by systematically altering the data address of a "load distributor" order which is carried in the upper accumulator; the variable instruction address of this order refers to a "store distributor" order.

Each block is entered with the point (x_o, y_o, z_o) which is the "origin point". The program then systematically raises these coordinates to (x_o, y_o+3, z_o+3) for the first plane, after which x_o is raised to (x_o+1) etc. to compute four planes of sixteen points each, or a total or sixty-four points for the block.

The four cosine sections compute the functions

$$\cos 2\pi(hx + ky + \ell z \pm \alpha),$$
$$\cos 2\pi(-hx - ky + \ell z \pm \alpha),$$
$$\cos 2\pi(hx - ky + \ell z \pm \alpha),$$
$$\cos 2\pi(-hx + ky + \ell z \pm \alpha).$$

This feature permits greater speed, if the crystal possesses symmetry such that $F(hk\ell)$ is the same for two or more of these permutations; in such cases, the cosines are summed algebraically before multiplication, so that fewer lengthy multiplications need be done.

Section 5 carries out the algebraic summation of cosines (provision is made for altering the sign of the cosines in each permutation) and the multiplication by $F(hk\ell)$. This product is then added to the partial sum for the previous reflections and stored. In centrosymmetric cases, $F(hk\ell)$ rather than $|F(hk\ell)|$ can be used.

Section 6 contains the procedure, necessary at the end of each plane, for raising the x-coordinate for the cosine blocks and altering various constants for section 5.

Section 7 is the routine referred to immediately after reading a detail card with new F, h, k, ℓ, and α'. It sets up the initial angles for sections 1-4 and initializes the constants necessary to pass from one point to the next higher within a line, and from one line to the next higher within a plane.

Section 8 modifies the orders which pick up cosines in section 5, inserting an "add lower" order if F(hkℓ) is to be added in a given permutation, "a subtract lower" if it is to be subtracted and a "no-op" if that permutation was not computed in a given problem. This section functions only upon reading of a special "modification card" (See "Detailed Operating Instructions") which gives the necessary orders to be entered for the ensuing class of reflections. Section 8 also inserts the proper signs for α', the phase angle, in each permutation; the orders for this purpose are read from a second modification card. This second card is omitted if $\alpha' = 0$.

Section 9 punches out the sixty-four final sums, on eight cards, after completion of the program. It is loaded only at the end of the program because of insufficient drum space, but the punch routine loads into erasable storage and does not affect the subsequent use of the main program for additional blocks. Section 9 must, however, be reloaded at the end of each new block. Each storage whose contents are punched is cleared to zero. The routine computes and punches plane number and range for each output card.

2. Range and accuracy

This is a fixed-point routine; the output cards contain six digits of each final sum with the scale of the results shifted the same amount as the $F(hk\ell)$ if a scaling factor is introduced. The indices h and k may have values from -39 to +39, and ℓ from 0 to 39. x_o, y_o, and z_o run from 0 to 80.

3. Storage

The block program uses the entire two-thousand words of drum storage. Of these, about two-hundred are temporary storages which may be used between reflections.

4. Speed

The program computes, on the average, about twenty detail cards per minute.

5. Equipment specifications

The basic I.B.M. 650 is required, with two-thousand words of drum storage. No special attachments to the machine are used.

6. Error checks

Storage 0000 contains an order which stops the machine if any of the instructions were not loaded onto the drum. The routine contains no other built-in error checks; however the procedure can be checked by running overlapping blocks if machine errors are suspected.

7. Input-output

The format of input and output cards is discussed in more detail under "Detailed Operating Instructions". Input consists of detail cards containing $F(hk\ell)$, h, k, ℓ, α', special load cards specifying origin of block, permutations to be computed, and signs for $|F(hk\ell)|$ and phase angles in the different permutations. These special cards are multiple-order load cards which are read into 1951-1958. The detail cards are entered by board wiring and cause the program to start at the instruction address of the console, which is the first order of section 7. The detail card format may also be used for the Least Squares II calculation.

Output consists of eight punched cards each of which has the eight final sums for half of one plane. Plane number and range are punched in each card, as is the origin of the block, x_o, y_o, z_o.

8. Symmetry provisions

The form of the expression actually calculated is

$$\rho(xyz) = \sum_{hk\ell\ 0}^{\infty} |F'(hk\ell)| \Big[\pm \cos 2\pi\,[hx + ky + \ell z \pm \alpha(hk\ell)] \pm \cos 2\pi\,[-hx - ky + \ell z \pm \alpha(\bar{h}\bar{k}\ell)] \pm \cos 2\pi\,[hx - ky + \ell z \pm \alpha(h\bar{k}\ell)] \pm \cos 2\pi\,[-hx + ky + \ell z \pm \alpha(\bar{h}k\ell)]\Big]$$

where F' represents structure factors divided by the proper factors required to take into account the differing multiplicities of non-general reflections.

$\alpha(hk\ell)$ must be an integral multiple of 1/80. If desired $F(hk\ell)$ instead of $|F(hk\ell)|$ can be used with no change in the program in the case of a center of symmetry. The program handles h and k algebraically. It also calculates any one or all of the permutations. If the algebraic form of the expressions does not change, the + and - index terms may be computed without modification by actually computing for negative indices. Modification cards are inserted between groups of reflections when the form must be changed.

B. Detailed Operating Instructions

1. Detail cards

One detail card is punched for each reflection, in the form hh kk$\ell\ell$ ab00 00 0000 0000 00 00OF FFFF 00 0000 0000 00 0000 $\alpha'\alpha'\alpha'\alpha'$ 00 0000 0000 00 0000 0000 00 0000 00c0 , where a = sign of h, b = sign of k and c = sign of $F(hk\ell)$.

α' is expressed as n/80 (4000) where n = 0,1,...,79 and $n = \frac{80\,\alpha}{2\pi}$. α = phase angle in radians and is so chosen as to give integral n.

At the beginning of program, the read band contains the following:

1951	00	0000	0000	,
1952	00	00hh	0000	,
1953	00	00kk	0000	,
1954	00	00$\ell\ell$	0000	,
1955	00	FFFF	F000	,
1956	00	$\alpha'\alpha'\alpha'\alpha'$	0000	,
1957-1960	00	0000	0000	.

2. Special information cards

Special information cards are load cards and should have a Y-punch in the column used to identify load cards.

a. Switch cards There may be one, two or three of these cards which tell the program which permutations to compute. They are single-order load cards of form:

```
            Y                          Y              Y
69 1954 1953  00 0000 0000  24 XXXX 8000  00 0000 ZZZZ
```

where XXXX is one of the program section 1, 2, or 3 exits. These exits are 0994, 0284 or 0800 respectively. ZZZZ is the address of the next permutation to be computed.

If next desired section is 2 $(-hx - ky + \ell z \pm \alpha)$, then

ZZZZ = 0934.

If next desired section is 3 $(hx - ky + \ell z \pm \alpha)$, then

ZZZZ = 0100.

If next desired section is 4 $(-hx + ky + \ell z \pm \alpha)$, then

ZZZZ = 0318.

If next desired section is 5 (Sum. and Mult.), then

ZZZZ = 1301.

b. <u>Origin card</u> The origin card contains starting coordinates, x_o, y_o, z_o in units of 1/80th of the unit cell with instructions for storing them. This card has the form

69 1956 195$\overset{Y}{2}$ 24 1460 195$\overset{Y}{3}$ 69 1957 195$\overset{Y}{4}$ 24 1234 195$\overset{Y}{5}$
69 1958 122$\overset{Y}{6}$ 00 0000 $00X_o\overset{Y}{X}_o$ 00 0000 $00Y_o\overset{Y}{Y}_o$
00 0000 $00Z_o\overset{Y}{Z}_o$.

c. <u>Modification cards</u> The modification cards contain the desired pick-up orders for the summation routine with orders for storing them, and also pick-up orders for the phase angle. The operation codes are 15 or 16 except for the first permutation used, in the first modification card. The codes used here must be 65 or 66.

The first modification card has the form 00 0000 007$\overset{Y}{9}$
aa 0027 008$\overset{Y}{1}$ bb 1027 133$\overset{Y}{4}$ cc 1077 048$\overset{Y}{4}$ dd 0077 073$\overset{Y}{1}$
00 0000 0000 00 0000 0000 00 0000 0000 , where aa, bb, cc, and dd are operation codes for the first, second, third and fourth permutations respectively.

The second modification card controls the sign of the α' term in the argument of the cosine. This card is used only when α' is not zero and has the form 00 0000 143$\overset{Y}{2}$
ee 1956 018$\overset{Y}{2}$ bb 1956 151$\overset{Y}{3}$ gg 1956 086$\overset{Y}{7}$ 69 1956 195$\overset{Y}{7}$
hh 1956 051$\overset{Y}{3}$ 24 0148 800$\overset{Y}{0}$ 00 0000 0000 , where ee, bb, gg, and hh are operation codes for the first through the fourth permutations.

3. <u>Program loading cards</u>

These cards are placed in front of the program deck and are used to zero the magnetic drum and to load the loading routine. These cards must be kept in the order below.

Card 1 is

```
Y          Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 0000 8000  00 0000 8000
           Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 2 is

```
Y          Y             Y             Y             Y
69 1952 1953  00 0001 0000  24 0001 1954  69 1955 1956
           Y             Y             Y             Y
10 0001 8003  24 0002 1957  61 1958 8003  20 1999 0002  .
```

Card 3 is

```
Y          Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 0000 8000  01 0000 8000
           Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 4 is

```
Y          Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 1082 8000  70 1950 1418
           Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 5 is

```
Y          Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 1950 8000  69 1952 1951
           Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 6 is

```
Y          Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 1157 8000  69 1954 1953
           Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 7 is

```
Y         Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 1613 8000  69 1956 1955
          Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

Card 8 is

```
Y         Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 1884 1082  69 1958 1957
          Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

The format of the four order load cards is

```
Y         Y             Y             Y             Y
24 XXXX 1645  XX XXXX XXXX  24 XXXX 1695  XX XXXX XXXX
          Y             Y             Y             Y
24 XXXX 1745  XX XXXX XXXX  24 XXXX 0985  XX XXXX XXXX  ,
```

where the X's correspond to addresses and orders to be loaded. A transfer from the four order loading routine is made by punching the I address of the last store order on the last card with 8000.

The punching routine is loaded by single order load cards of the form

```
Y         Y             Y             Y             Y
69 1954 1953  00 0000 0000  24 XXXX 8000  XX XXXX XXXX
          Y             Y             Y             Y
00 0000 0000  00 0000 0000  00 0000 0000  00 0000 0000  .
```

The exit from this loading procedure is accomplished by a load card punched with

```
Y         Y
00 0000 0009
```

in the first field.

4. Output cards

Two cards are punched for each of four planes. The first such card, identified by a 1 in. col. 1, contains final sums for points in the first two lines of the plane. These are punched in order of increasing Z coordinate, in the following format:

Cols.	
1	Range number (1 or 2, for 1st, 2nd half-plane),
2	Plane number,
3,4	x_o,
5,6	y_o,
7,8	z_o,
13-18	Sum for x_o, y_o, z_o,
19-24	Sum for x_o, y_o, $(z_o + 1)$,
25-30	Sum for x_o, y_o, $(z_o + 2)$,
31-36	Sum for x_o, y_o, $(z_o + 3)$,
37-42	Sum for x_o, $(y_o + 1)$, z_o,
43-48	Sum for x_o, $(y_o + 1)$, $z_o + 1$,
49-54	Sum for x_o, $(y_o + 1)$, $z_o + 2$,
55-60	Sum for x_o, $(y_o + 1)$, $z_o + 3$.

The second card of each plane has final sums for the last two lines of the plane also arranged with increasing z's.

5. Operating procedure

Console should be set to 70 1951 1418. Sense switches and programmed stop switch are set to "stop". First two cards are a drum-clear routine for use with this console setting. They clear the entire drum to minus zeroes before loading in the four-order program load cards. Origin card is placed directly behind the program desk, followed by the switch cards, then the two modification cards associated with the first class of reflections to be computed. Each new class of reflections must have these two modification cards in front of its detail cards. The detail cards go in after the special cards; they should be sorted on ℓ because considerable time can be saved whenever ℓ does not change between cards. The punch program is behind the last detail card. When the block is completed the machine will return to the console to read new origin card etc., for the next block. If no additional cards are in the card reader, program will stop on "input-output".

6. Flow diagram, program cards, and wiring diagram

The flow diagram for the T.D.F. 80 B program is given in Figure 3. The wiring diagram is given in Figure 4. The program cards are listed in Table 13. The quantities listed are the addresses and the orders. These must be made up into four-order load cards. The punch routine orders are listed in Table 14. These form single order load cards.

Section 7. 8000 7019511418
Read detail card and initialize point and line constants for the first plane

Section 9.
0009 6514600027
Punch routine.

end.

Section 1. 0428 6007810087
cos $2\pi(hx + ky + \ell z \pm \alpha)$.

Switchcard in 0994.

Section 2. 0934 6003400545
cos $2\pi(-hx - ky + \ell z \pm \alpha)$.

Section 8.
0079 6001320989
Modify pickup orders.

Switchcard in 0284.

Section 3. 0100 6000640669
cos $2\pi(hx- ky + \ell z \pm \alpha)$.

Switchcard in 0800.

Section 4. 0318 6005280084
cos $2\pi(-hx + ky + \ell z \pm \alpha)$.

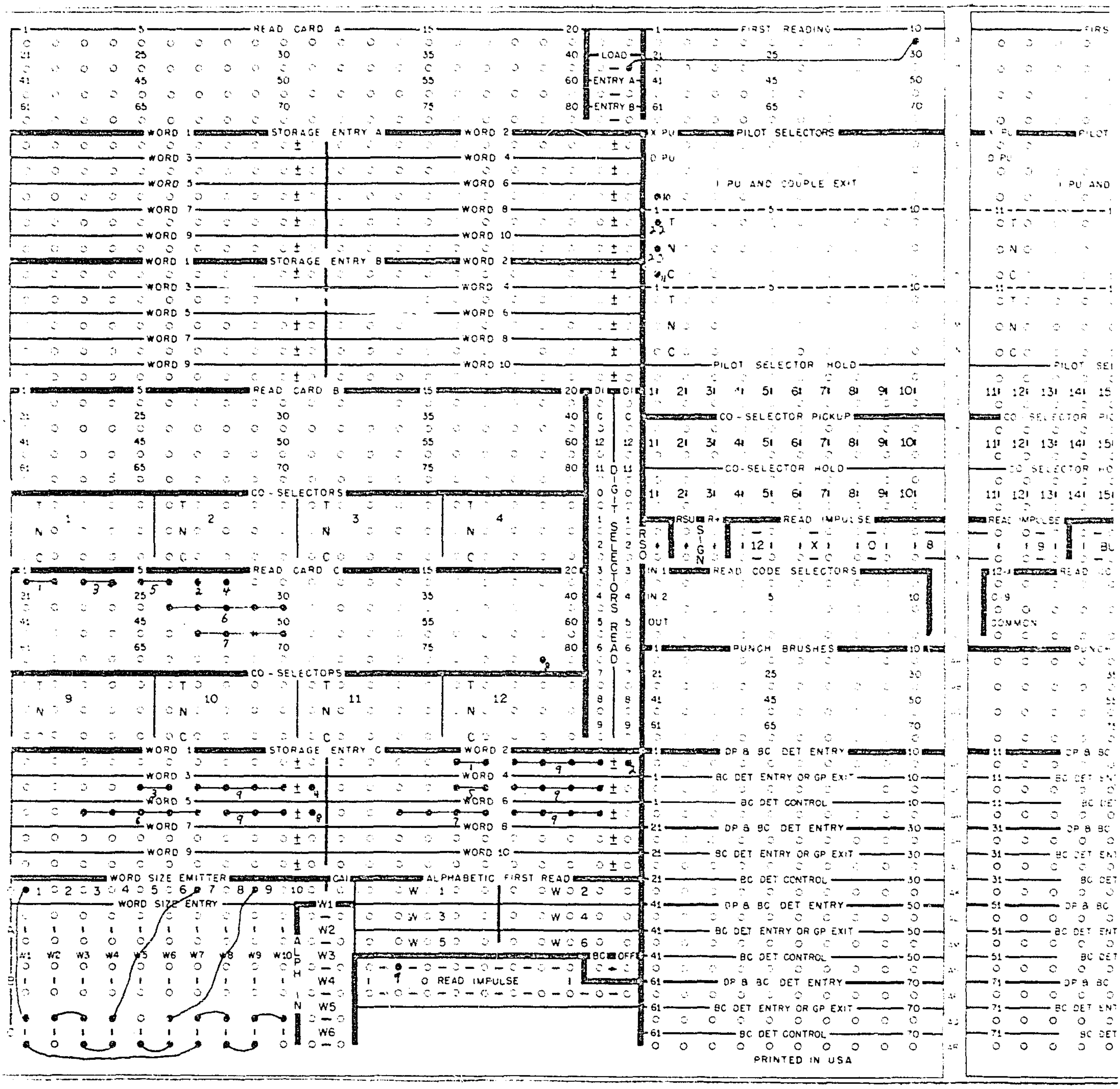
Section 5. 1301 6500090014
Multiplication and formation of partial sums.

Test end of block.

Section 6. 1876 1505790534
Initialize plane and line constants and raise starting angles.

Figure 3. Flow diagram for T.D.F. 80 B program

Figure 4. T.D.F. 80 B wiring diagram for the I.B.M. 650


READ CARD A
LOAD
ENTRY A
ENTRY B
FIRST READING
STORAGE ENTRY A
PILOT SELECTORS
X PU
D PU
I PU AND COUPLE EXIT
STORAGE ENTRY B
PILOT SELECTOR HOLD
READ CARD B
CO - SELECTOR PICKUP
CO - SELECTOR HOLD
CO - SELECTORS
DIGIT SELECTORS READ
READ IMPULSE
READ CARD C
READ CODE SELECTORS
PUNCH BRUSHES
STORAGE ENTRY C
DP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
WORD SIZE EMITTER
WORD SIZE ENTRY
ALPHABETIC FIRST READ
READ IMPULSE
PRINTED IN USA

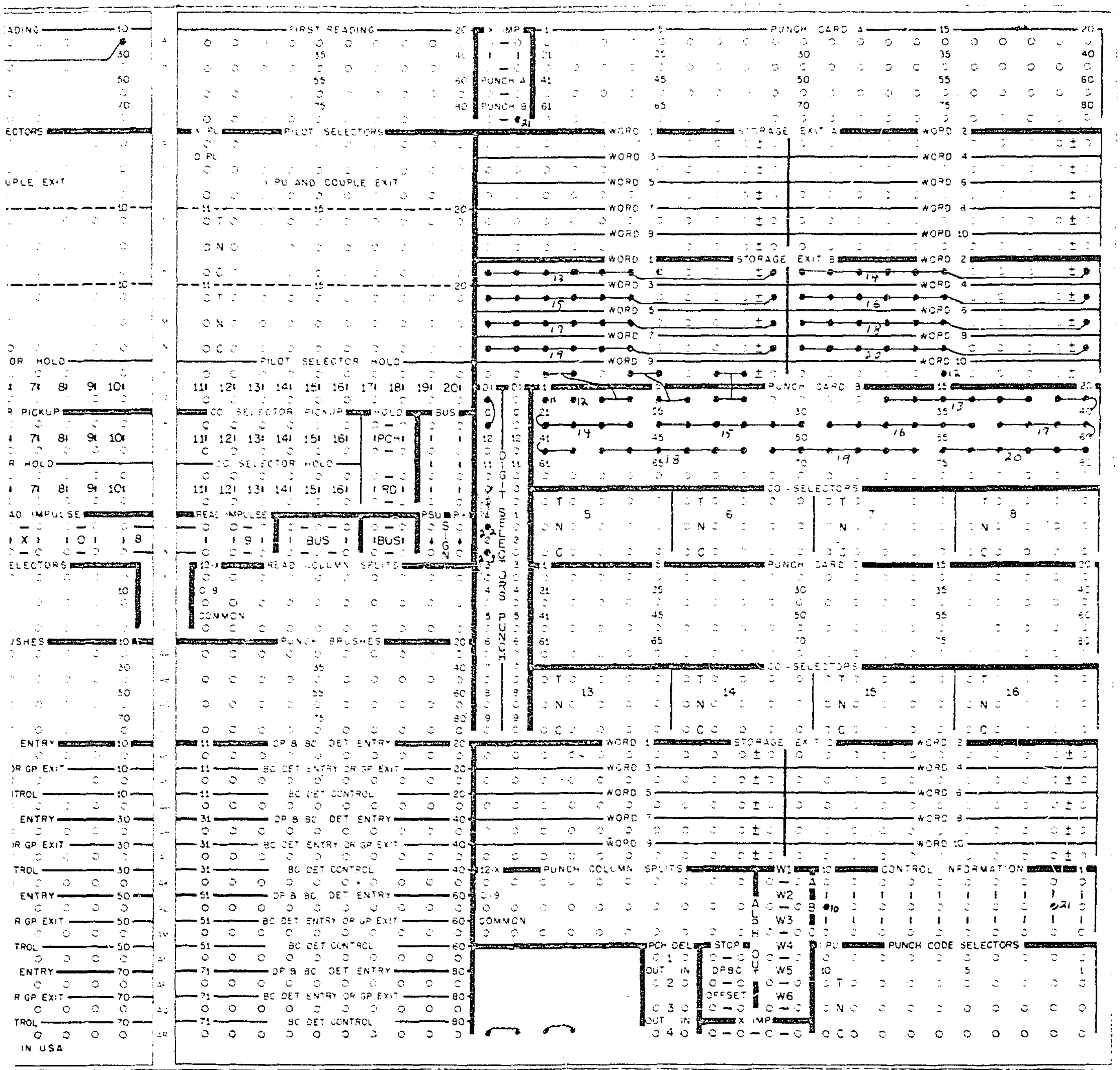

FIRST READING
PUNCH CARD A
PUNCH A
PUNCH B
PILOT SELECTORS
STORAGE EXIT A
STORAGE EXIT B
PU AND COUPLE EXIT
PILOT SELECTOR HOLD
PUNCH CARD B
CO - SELECTOR PICKUP
CO - SELECTOR HOLD
READ IMPULSE
BUS
READ COLUMN SPLITS
COMMON
PUNCH BRUSHES
CO - SELECTORS
PUNCH CARD C
DIGIT SELECTORS
OP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
STORAGE EXIT C
PUNCH COLUMN SPLITS
CONTROL INFORMATION
PUNCH CODE SELECTORS
PCH DEL
STOP
DPBC
OFFSET
X IMP
IN USA

TABLE 13. PROGRAM ORDERS FOR T.D.F. 80 B (SYMBOLS
* AND ⌑ REPRESENT X/O AND Y/O)

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0001692020027C	0002099999999I	0003099999999R	0004460007015H
0005241359156B	0006241359161B	0007100010800C	0008100011800C
0010692020032C	0011690021037D	0012111315001I	0013690020067C
0016690036058I	0017101627800C	0018690036183I	0019460022172E
0020099999999I	0022100025800C	0023241127073⌑	0024241127078⌑
0025692035043H	0026000482043C	0028690036033I	0029460482069G
0030110633003G	0031000083997H	0032200147150⌑	0035099999999I
0036099999999R	0037460040009A	0038241342009E	0039241342009F
0040101943800C	0041100044800C	0043692002065E	0044690003065F
0045110899000D	0046110749125E	0047200551021C	0048161656186A
0050100254800C	0051151805180I	0052099691733D	0053099691733M
0054460057030H	0055240109016B	0056240109021B	0057100060800C
0058100061800C	0060692020062C	0061690021042D	0062111365141I
0063690021032D	0066111926078B	0067000014046D	0068690947060⌑
0069460122192E	0070099691733D	0071099691733M	0072101376800C
0073241277143⌑	0074241277148⌑	0075692035058H	0076441929073B
0078690036043I	0079600132098I	0080110683143G	0082004000000⌑
0084460890084A	0085099691733D	0086099691733M	0087460090004A
0088241192094E	0089241192024F	0090100043800C	0091100094800C
0093692002035E	0094690003005F	0095110099050D	0096110049130E
0097161810021F	0100600064066I	0101100000019E	0102098768834A
0103098768834J	0104460107071F	0105241209101B	0106241209106B
0107100110800C	0108101868800C	0110692020092C	0111690021007D
0112111165196I	0113690020007C	0116461690149A	0117692036183I
0118000000000⌑	0119460172092E	0120098768834A	0121098768834J
0122100075800C	0123240377193⌑	0124240377013⌑	0125692035088H
0126692036033I	0128690036078I	0129100346800C	0130110283118G
0131240698800C	0132201217122H	0134002000000⌑	0135098768834A
0136098768834J	0137460140014A	0138240242024E	0139240242029E
0140100093800C	0141100144800C	0143692002080E	0144690003035F
0145111199005D	0146110949135E	0148151956051C	0150151956086G
0151691410156D	0152097236992⌑	0153097236992*	0154460157065H
0155240159026B	0156240159051B	0157100160800C	0158100063800C
0160692020017C	0161690021147D	0162110115006I	0163690020107C
0164160067032H	0166460440067H	0168100628800C	0169461822167D
0170097236992⌑	0171097236992*	0172100175800C	0173240327038⌑
0174240327043⌑	0175692035013H	0176692036108I	0178690036013I
0179240698800C	0180111233013G	0182100892059G	0184460122024H
0185097236992⌑	0186097236992*	0187460190019A	0188240292065A
0189240292069F	0190100143800C	0191100194800C	0193692002020E
0194690003080F	0196111049140E	0197461750135D	0200691106185I
0201190354134A	0202095105651F	0203095105651O	0204460207060I
0205240409056B	0206240409061B	0207100210800C	0208100161800C
0210692020022C	0211690021052D	0212110165146I	0213161368003B

TABLE 13. CONTINUED

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0216461874037H	0217240021133B	0218240981123I	0219460222137C
0220095105651F	0221095105651O	0222100125800C	0223240427053¤
0224240427058¤	0225692035023H	0226690035003H	0228200581108D
0229200884133I	0230111283148G	0231200514075G	0232200340186¤
0234191788030¤	0235095105651F	0236095105651O	0237460240045¤
0238240442044E	0239240442059F	0240100193800C	0241100944800C
0243692002175E	0244110401026F	0245110299010D	0246110149145E
0247201805031C	0248100016800C	0250460422186D	0251016000000¤
0252092387953B	0253092387953K	0254690021027D	0255241009076B
0256241009046C	0257100260800C	0258100211800C	0260692020002C
0261690021062D	0262110315101I	0263690020052C	0264151679191G
0266461672117D	0267650781143H	0268460740069A	0269460272167C
0270092387953B	0271092387953K	0272100225800C	0273241027063¤
0274241027068¤	0275692035028H	0276692036078I	0278451831118B
0279211195128D	0280111833018G	0282110147155¤	0285092387953B
0286092387953K	0287460290029A	0288241042059E	0289241042064E
0290100243800C	0291100294800C	0293692002025E	0294690003105F
0295110249175D	0296111249190E	0297241805185H	0300201807166D
0301651807096C	0302089100652D	0303089100652M	0304460257070I
0305241109091B	0306241109096B	0307100310800C	0308100261800C
0310692020037C	0311211695151G	0312110715011I	0313200118800¤
0316161824082I	0317000000005¤	0318600528008D	0319460972172D
0320089100652D	0321089100652M	0322100275800C	0323240027003¤
0324240027008¤	0325692035033H	0326690035083H	0328201983163H
0329211495148D	0330111883183G	0331201801125G	0332690002060E
0334690020002C	0335089100652D	0336089100652M	0337460840079A
0338241142069E	0339241142049E	0341100344800C	0343692002030E
0344690003025F	0345111799015D	0346690002020E	0347450200015A
0348110401016F	0350101967800C	0351200340030A	0352085264016D
0353085264016M	0355240209031B	0356240209036B	0357100360800C
0358100861800C	0360692020042C	0361690020082C	0362110765151I
0363692035183H	0364151817800C	0366190726036H	0367002000000¤
0368200478138A	0369460322112C	0370085264016D	0371085264016M
0372100325800C	0373241227083¤	0374241227048¤	0375692035038H
0376690036088I	0378160082019G	0379211645158D	0380110333023G
0382240842100¤	0384651656066F	0385085264016D	0386085264016M
0387460390034A	0388241242074E	0389241242004F	0390100293800C
0391101494800C	0393692002010E	0394110401046F	0395111749180D
0396110849165D	0397241805118D	0400690020092C	0401002000000¤
0402080901699D	0403080901699M	0404460307000H	0405241309111B
0406241309116B	0407100410800C	0408100111800C	0410692020047C
0411690021047D	0412111615021I	0413160167152I	0416111926058B
0418161926023B	0419461273127E	0420080901699D	0421080901699M
0422100375800C	0423241327093¤	0424241327098¤	0425692035003H
0428600781008G	0429211795168D	0430110383158G	0431201001096F

TABLE 13. CONTINUED

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0441100444800C	0443692002040E	0444690003010F	0445110499020D
0446111149170D	0447150401165E	0448100001800C	0450111207061C
0451201810126D	0452076040596F	0453076040596O	0454460357005H
0455241409121B	0456241409126B	0457100460800C	0458100461800C
0460692020142C	0461690021067D	0462111665156I	0463110565166I
0466461558160I	0467101173800C	0468151375162I	0469460372162E
0470076040596F	0471076040596O	0472100425800C	0473241427103□
0474241427108□	0475692035048H	0476690036023I	0479211945150D
0480110783178G	0482151488069G	0485076040596F	0486076040596O
0487460490044A	0488241442084E	0489241442014F	0490100393800C
0491100494800C	0493692002045E	0494690003040F	0495110649120E
0496111349130D	0497201949160D	0500064000000□	0502070710678A
0503070710678J	0504460407176D	0505241059131B	0506241059136B
0507100510800C	0508100761800C	0510692020052C	0511690021072D
0512110365131I	0513150167063B	0516111926093B	0518461007160H
0519460422024D	0520070710678A	0521070710678J	0522100475800C
0523241077123□	0524241077128□	0525692035053H	0526650429043D
0527690035063H	0529201834105□	0530110433028G	0532151639084G
0534451938118I	0535070710678A	0536070710678J	0537460540049A
0538241092089E	0539241092019F	0540100443800C	0541100544800C
0542200499110E	0543692002050E	0544690003045F	0545460448005□
0546111549185E	0548461473001G	0550460922061F	0552064944804H
0553064944804Q	0554460457020H	0555241159141B	0556241159011B
0557100560800C	0558650311196E	0560692020057C	0561690021077D
0562110415026I	0563160367167E	0564160082099H	0566461090127H
0567241675800C	0568110021007F	0569460472122C	0570064944804H
0571064944804Q	0572100525800C	0573241177133□	0574241177138□
0575692035008H	0576690036028I	0577690036053I	0578200215182I
0579000001000□	0580110483163G	0582460407115A	0585064944804H
0586064944804Q	0587460590054A	0588240142014E	0589240142044F
0590100493800C	0591200195199H	0592151095199I	0593692002055E
0594690003050F	0595110599030D	0596110449115E	0597211953135F
0598460772191H	0600241675135F	0602058778525B	0603058778525K
0604460507025H	0605241259146B	0606241259151B	0607100610800C
0608151863111G	0609101962800C	0610692020007C	0611000033008D
0612110465161I	0613461140012I	0614690718147H	0616101328800C
0618461340194B	0619460522097C	0620058778525B	0621058778525K
0622100575800C	0623240127018□	0624240127023□	0625692035063H
0626690036003I	0627690035018H	0628690003020F	0629150478015□
0630110533038G	0631600878193D	0632151807146D	0634151956151C
0635058778525B	0636058778525K	0637461640104A	0638241292099E
0639241292029F	0640100543800C	0641100594800C	0642151679089G
0643692002060E	0644690003055F	0645110549185D	0646111649105D

TABLE 13. CONTINUED

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0647160500121F	0648461022102C	0650201656170I	0651110399095D
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0656240009006B	0657100910800C	0658100661800C	0659100113800C
0660692020067C	0661690021017D	0662111865041I	0663690020077C
0664201972162F	0666100878158I	0667461990092H	0668690036073I
0669460572102D	0670052249856E	0671052249856N	0672100625800C
0673241377153¤	0674241377158¤	0675692035068H	0676650479043D
0677690036008I	0678100832800C	0679201742049G	0680110583168G
0681692036048I	0682000031993B	0685052249856E	0686052249856N
0687460640064A	0688241392099F	0689241392049F	0690100593800C
0691100694800C	0692000018006G	0693692002000E	0694690003060F
0695110699040D	0696110349100D	0697160251160E	0698440951130F
0700151953061D	0702045399050¤	0703045399050*	0704460607040H
0705241459166B	0706241459171B	0707100660800C	0708100711800C
0709100862800C	0710692020072C	0711690021082D	0712111815111I
0713201267122H	0714690918013A	0716110729098D	0718441582140F
0719460622192D	0720045399050¤	0721045399050*	0722100675800C
0723241477163¤	0724241477168¤	0725692035073H	0728110134054H
0729002000000¤	0730110033043G	0731201141174D	0732101989180F
0734000015946B	0735045399050¤	0736045399050*	0737460690189A
0738241492199E	0739241492199F	0740100643800C	0741101094800C
0742110401056F	0743692002070E	0744690003070F	0745110799045D
0746111849115D	0747211445150A	0748200354130G	0750000068047¤
0751101454800C	0752038268343B	0753038268343K	0754460707045H
0755240059176B	0756240059181B	0757600713076H	0758111863051H
0759100013800C	0760692020077C	0761692021137D	0762110515036I
0763200167120¤	0764201972167F	0766241729176F	0767690036038I
0768691678187I	0769460672177D	0770038268343B	0771038268343K
0772100725800C	0773240077173¤	0774240077178¤	0775692035108H
0776650379043D	0777690036063I	0778110134059H	0779241675038D
0780110083173G	0782460107075A	0785038268343B	0786038268343K
0787460740074B	0788240092127I	0789240092054F	0790100693800C
0791100744800C	0792110401026H	0793692002075E	0794690003075F
0795690002000E	0796200033079G	0797150850095I	0798161922057H
0802030901699D	0803030901699M	0804461757180H	0805240309041B
0806240309046B	0807100760800C	0808100811800C	0809101163800C
0810692020082C	0811690021012D	0812690021137D	0813690818017I
0814200781183B	0816000016986H	0818441576145F	0819460722152C
0820030901699D	0821030901699M	0822100775800C	0823240177183¤
0824240177188¤	0825692035078H	0826690035043H	0827690035093H
0828110134055¤	0829460532084G	0830110733048G	0831201141199D
0832690003030F	0834461372177C	0835030901699D	0836030901699M
0837460790074A	0838240192104E	0839240192064F	0840100743800C
0841100794800C	0842201684133I	0843692002015E	0844690003015F
0845110999055D	0846161656022H	0847161800190D	0848200354095H

TABLE 13. CONTINUED

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0858100361800C	0859101063800C	0860692020087C	0861692021007D
0862690021002D	0863150118197C	0864201972172F	0866111926098B
0867460642089G	0868690229038B	0869460772072H	0870023344536D
0871023344536M	0872100825800C	0873240277113⌑	0874240277118⌑
0875692036083I	0876690035058H	0877690036068I	0878000000000C
0879211345138D	0880111983193I	0881690035048H	0882461408191⌑
0885023344536D	0886023344536M	0887460990039A	0888240342034E
0889240342039E	0890100793800C	0891100844800C	0892099691733D
0893692002085E	0894690003085F	0895111099060D	0896160401135G
0897691100111F	0898110401066G	0900111899110D	0902015643446E
0903015643446N	0904460857070H	0905240359071B	0906240359066B
0907100860800C	0908100911800C	0909101813800C	0910692021082D
0911690020012C	0912110615046I	0913690020002C	0914460240016H
0916000515051G	0917191972165G	0918441631160F	0919460822107D
0920015643446E	0921015643446N	0922100975800C	0923240227028⌑
0924240227033⌑	0925100178800C	0926690035013H	0927690035078H
0928101682800C	0929240634173I	0930110833053G	0931201141189D
0932460557158H	0934600340054E	0935015643446E	0936015643446N
0937460940089A	0938240392090⌑	0939240392074F	0940100843800C
0941100894800C	0942200499110F	0943692002090E	0944690002050E
0945110199065D	0946000017001G	0947200528153A	0948200354185G
0950151954081C	0951101256036D	0952007845909F	0953007845909O
0954460907075H	0955240459171D	0956240459121D	0957100960800C
0958650961196E	0959200083079H	0960692020012C	0961211395131G
0962110665171I	0963160167062I	0964201972077F	0966691382117I
0967151679006H	0968241675135F	0969460872112D	0970007845909F
0971007845909O	0972100276800C	0973101028800C	0974101777800C
0975692035083H	0976241563021H	0976241563021H	0977690036108I
0978101132800C	0980110883153G	0982460907168I	0984461507178I
0985007845909F	0986007845909O	0987000000000⌑	0988160946085A
0989151952800C	0990101043800C	0991101828800C	0992240698800⌑
0993692002095E	0995111299070D	0996111399075D	0997110401011F
0998461251105E	1000151955071D	1002000000000⌑	1003000000000⌑
1004461007086F	1005000031948⌑	1005000031948⌑	1006161963046G
1007101260800C	1008101011800C	1010151863171G	1011690020032C
1012110215051I	1013110816800C	1014461067041H	1016101128800C
1017000000000⌑	1018241150170F	1019460922122D	1020000000000⌑
1021000000000⌑	1022100875800C	1023100326800C	1024100577800C
1025101378800C	1026690035088H	1028690036048I	1029692003190F
1030110933058G	1031201141194D	1032240987118D	1034692035023H
1035000000000⌑	1036000000000⌑	1037461790094A	1038161441114F
1039100542004H	1040100943800C	1041101044800C	1043692003015F
1044690002085E	1045111699090D	1046111450155E	1047211295140A

TABLE 13. CONTINUED

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1057101816800C	1058101061800C	1060692021032D	1061690020062C
1062110265176I	1063690020022C	1064201972052F	1066101079800C
1067151926023B	1068201999110F	1069461072132D	1070007845909O
1071007845909F	1072101125800C	1073240477028B	1074100977800C
1075690002095E	1076690035023H	1078692002190F	1079690002190F
1080110983188G	1084151138174C	1085007845909O	1086007845909F
1087461040099A	1088241592080¤	1089241592080¤	1090101993800C
1091101144800C	1093692003085F	1094690003000F	1095004000000¤
1096110551187H	1097211745170A	1098160401170E	1099692035053H
1100200064176G	1101150916052I	1102015643446N	1103015643446E
1104460957080H	1105161908151D	1106000001000¤	1107000003000¤
1108651161196E	1110692021062D	1111690020017C	1112110815056I
1113200014122H	1114190317152H	1116241675135F	1117200781188H
1119461222102E	1120015643446N	1121015643446E	1122101326800C
1123100576800C	1124100128800C	1125692035018H	1126690035028H
1128690003190F	1130111733108G	1131201141184D	1132200099110E
1134151138004G	1135015643446N	1136015643446E	1137461990169A
1138000033088C	1140101193800C	1143692003090F	1144690002070E
1145161949155D	1146110750800C	1147211895180A	1148200354110H
1150151956018B	1151100411800C	1152023344536M	1153023344536D
1154461057090H	1155461208085I	1156601460036F	1158101111800C
1160692021092D	1161211845161G	1162110865181I	1163690020042C
1164201972067F	1166000482043C	1167099691733M	1169460072152D
1170023344536M	1171023344536D	1172101476800C	1173000034003B
1174101877800C	1175692035093H	1176110729018D	1178200987024G
1179240842196D	1180111783128G	1181240842070¤	1182651538084F
1184650340114E	1185023344536M	1186023344536D	1187461340089H
1189691642029G	1190101243800C	1193692003020F	1194690002090E
1200601954161D	1201690021057D	1202030901699M	1203030901699D
1204221657136¤	1205461308090I	1206150611101C	1207002000000¤
1208101211800C	1210692021017D	1211692021022D	1212110915061I
1213690020047C	1214111081188I	1216461660126F	1218200183190¤
1219461473077H	1220030901699M	1221030901699D	1222101175800C
1223100626800C	1224110134064H	1225692036043I	1226241788800¤
1228100031193B	1229240987135¤	1230111033068G	1231150334079F
1235030901699M	1236030901699D	1237461090079B	1238151941800C
1239240547188B	1240101493800C	1241101294800C	1243692003070F
1244690002005E	1250191810076C	1251150367123A	1252038268343K
1253038268343B	1254690021087D	1255461358080I	1256201717122I
1257601113186G	1258100913800C	1260692021087D	1261692021002D
1262110965186I	1263690020142C	1264651167162H	1266161825002I
1269461272097D	1270038268343K	1271038268343B	1272100176800C
1273101526800C	1274101927800C	1275100827800C	1276692036008I

TABLE 13. CONTINUED

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1289350001064G	1290101143800C	1291101344800C	1293692003000F
1294690002035E	1300240021168H	1302045399050*	1303045399050⌑
1304461658075I	1305461408041F	1306651952142I	1307651610196E
1308101361800C	1310100163800C	1311211545141G	1312111015071I
1313064000000⌑	1314691017161H	1316200149161F	1318200065042H
1319461022082H	1320045399050*	1321045399050⌑	1322101225800C
1323101126800C	1324101728800C	1325692036013I	1326692036063I
1328690036083I	1329000000995A	1330111133073G	1331691068177H
1332690942175F	1335045399050*	1336045399050⌑	1337461190109A
1338110842069H	1340101593800C	1343692003005F	1344690002080E
1350241805118D	1352052249856N	1353052249856E	1354161207140D
1355461458150I	1356300001131D	1357200064026G	1358101411800C
1360601563091G	1361692021037D	1362111065016I	1363690020057C
1364240150195E	1366150850121H	1368000016076F	1369461172142D
1370052249856N	1371052249856E	1372101976800C	1373100376800C
1374240477088⌑	1375000033003C	1376692036068I	1378690036093I
1379151166043A	1380111183198G	1381601234125⌑	1382201684133I
1385052249856N	1386052249856E	1387461590179A	1388221341139D
1389460592199I	1390101343800C	1391101444800C	1393692003035F
1394600547020A	1400100117800C	1402058778525K	1403058778525B
1404151707166A	1405461508155I	1406651953155F	1407101060800C
1408101461800C	1410000002000⌑	1411692021042D	1412111115076I
1413200417122H	1414161926148A	1418601952151⌑	1419461322172C
1420058778525K	1421058778525B	1422101325800C	1423241527028D
1424100627800C	1425692036088I	1426692036073I	1428200481133I
1429150026033A	1430110133078G	1431160134148I	1432691952101H
1435058778525K	1436058778525B	1437461390199A	1438151742109H
1440101393800C	1441000019001I	1443692003080F	1444690002175E
1452064944804Q	1453064944804H	1454690021092D	1455461558051F
1456651954110A	1457101110800C	1458101511800C	1461692021047D
1462111215081I	1463690020072C	1464460967006H	1466201767122I
1468200514122I	1469461372117F	1470064944804Q	1471064944804H
1472101425800C	1473101426800C	1474241527028D	1475150478115⌑
1476692036018I	1478240698800C	1479000016001F	1480110183123G
1481200528042H	1482000500050⌑	1485064944804Q	1486064944804H
1487461440124A	1488032000000⌑	1489461792089F	1490101443800C
1491101544800C	1493692003105F	1494690002015E	1500690814077I
1502070710678J	1503070710678A	1504661107086C	1505100018800C
1506461759176⌑	1507101160800C	1508101561800C	1509101263800C
1510190317138I	1511692021147D	1512111265116I	1513460264191G
1514111968800C	1516151810056D	1518200917122I	1519461422182C
1520070710678J	1521070710678A	1522101525800C	1523100877800C
1524101577800C	1525692036023I	1526692036093I	1528691581130⌑

TABLE 13. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
15291604780630D	1530111333083G	1531691955097F	1532200133136F
1535070710678J	1536070710678A	1537461540159A	1538692002095E
1540101543800C	1541101594800C	1542000018041H	1543692003040F
1544690002030E	1550461911101F	1552076040596O	1553076040596F
1554151207101D	1555460108177I	1556151482023A	1557101210800C
1558101611800C	1559100263800C	1561692021052D	1562110015086I
1564240118178A	1566161329163B	1569461472187C	1570076040596O
1571076040596F	1572101575800C	1573200727173A	1575692036028I
1576101466036D	1577690035068H	1578100881800C	1580111383138G
1581201815056I	1582101468036D	1585076040596O	1586076040596F
1587461140167G	1588101201800C	1589168002170¤	1590101293800C
1591101644800C	1593692003095F	1594690002010E	1600101029800C
1602080901699M	1603080901699D	1604601953111D	1605461758031F
1606651955137I	1607101261800C	1608101811800C	1609101363800C
1610211245121G	1611692021057D	1612110065121I	1614190317065¤
1616161479153B	1618220027043B	1619461522192C	1620080901699M
1621080901699D	1622100126800C	1623100226800C	1624200099171C
1625100028800C	1626650279043D	1627690035073H	1628201952115F
1629110734800C	1630111433033G	1631101518036D	1632200199166F
1635080901699M	1636080901699D	1637461240139A	1638161542165¤
1639008000000¤	1640101093800C	1641101694800C	1642000003000¤
1643692003030F	1644690002040E	1650201081113D	1652085264016M
1653085264016D	1654461407100H	1655461010141D	1658101914800C
1659100663800C	1660151313126F	1661691814021G	1662111415091I
1663690035183H	1664150167147E	1666150850131F	1669461572132C
1670085264016M	1671085264016D	1672101775800C	1673100476800C
1674101727800C	1675200781183B	1676650879043D	1677111207091D
1678201734133I	1679960000000¤	1680111483133G	1681200015185A
1682690003095F	1685085264016M	1686085264016D	1687460350196F
1688461842045A	1689101254800C	1690101643800C	1691111207061H
1692000001000¤	1693692003010F	1694690002045E	1700198001009G
1702089100652M	1703089100652D	1704461457105H	1705460608190I
1706691953092I	1707690035003H	1708101761800C	1709608002023D
1710002000000¤	1711692021072D	1712111465126I	1713150850176C
1714110581128H	1716000019006I	1717200528042H	1719461622127D
1720089100652M	1721089100652D	1722101875800C	1723100826800C
1724100927800C	1725100078800C	1726650329043D	1727690035008H
1728690036018I	1729002000000¤	1730111533093G	1731691784138H
1732200265177B	1735089100652M	1736089100652D	1737461690034H
1738100561800C	1739691954136D	1740101693800C	1741101794800C
1743201450016D	1744651047005A	1750151207140D	1752092387953K
1753092387953B	1754461507006F	1755240509099D	1756241933097H
1757100710800C	1758151961031F	1759101711800C	1760101463800C
1761692021077D	1762111515096I	1763200049156F	1764111926088B
1766200021133A	1767660478014H	1768161729178B	1769461672188A

TABLE 13. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1770092387953K	1771092387953B	1772150682162D	1773100876800C
1774100777800C	1775692036038I	1777690035108H	1778241933063A
1779100812800C	1780111583088G	1781240987039G	1782451931150¤
1784100000072G	1785092387953K	1786092387953B	1787461740154A
1789100400800C	1790100893800C	1791100795800C	1792150401135G
1793692003045F	1794690002055E	1800004000000¤	1802095105651O
1803095105651F	1804461557115H	1805000000000¤	1806161815027H
1808100511800C	1809201913191F	1811690020087C	1812111565031I
1813690020037C	1814200315056I	1816692021012D	1817000085008C
1818150726143A	1819461722162C	1820095105651O	1821095105651F
1822101276800C	1823100926800C	1824008000000¤	1825032000000¤
1826690002025E	1827100681800C	1828690003090F	1829150850173B
1971099691733D	1973451876117H	1974100527800C	1976692036058I
1985099691733M	1986099691733D	1987461940174A	1988191141197E
1989000000000A	1990100993800C	1991101244800C	1992100363800C
1997211595160A	1998690101120D	1999200726067I	1996111449150F
1830111633103G	1831651892105A	1832651807041C	1835095105651O
1836095105651F	1837461490129A	1838240492104F	1839240492109F
1840101793800C	1841101194800C	1842151095045A	1843692003050F
1844651147005A	1850440951130F	1851150850131H	1852097236992*
1853097236992¤	1854461607125H	1855461708165I	1857651311196E
1858240118103B	1859240118122I	1860650064181H	1861690814056G
1862111765136I	1863002000000¤	1864100767800C	1867691428118A
1868692020107C	1869461827157H	1870097236992*	1871097236992¤
1872221975192H	1873101026800C	1874150134140D	1875692036003I
1876150579053D	1877690035038H	1878460508131¤	1879240842095¤
1880111683063G	1881110134025¤	1882651656176H	1885097236992*
1886097236992¤	1887461840164A	1888650528128A	1889461400190A
1890101843800C	1891100644800C	1892099999999R	1893692003055F
1894651997005A	1900161716168A	1901101663800C	1902098768834J
1903098768834A	1904461907056C	1905460358065I	1906240559130A
1907151710167E	1908000015001E	1909161863111G	1910101213800C
1911101078800C	1912111715106I	1914692021067D	1916691919187B
1917690351096H	1918100668800C	1919100000191C	1920098768834J
1921098768834A	1922000018991I	1923101076800C	1924100677800C
1925110729083D	1926002000000¤	1927690035033H	1928600981198H
1929101933123H	1930110233113G	1931651034103I	1932160692800C
1933201999110F	1934191656151F	1935098768834J	1936098768834A
1937461890024A	1938151692034G	1939461600106F	1940101893800C
1941000033008C	1942101075800C	1943692002005E	1944651097005A
1952099691733M	1953099691733D	1961016000000¤	1962690021022D
1963000015001E	1964691850099B	1965150118157C	1966101826800C
1967692003025F	1968000066011G	1969461122197D	1970099691733M
1993692003060F	1994650747005A	1995111499080D	1996111449150F

TABLE 14. PROGRAM ORDERS FOR T.D.F. 80 B PUNCH (SYMBOLS * AND ¤ REPRESENT X/0 AND Y/0)

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0009	651460002G	0027	350003004B	0042	151234010I	0109	350003012G
0127	151788014B	0142	201985020I	0209	650059007G	0059	691195800C
0077	100092800B	0092	241977019B	0192	690227024B	0227	240000025I
0242	220277029B	0292	691017027G	0259	110309032G	0309	241984019C
0327	440342035I	0342	100377039B	0377	241985019C	0392	150409800B
0409	000050000¤	0359	101989042G	0427	160442055I	0442	001544000¤
0559	691009102G	1009	800000008¤	1027	221986104B	1042	150442105I
1059	711977107G	1077	150409109B	1092	100092110I	1109	691127114B
1127	440342115I	1142	240327800B	1159	101989147G	1477	161192120I
1192	001944000¤	1209	691227124B	1227	900000008¤	1242	221986125I
1259	151192127G	1277	711977129B	1292	161309135I	1309	691948800C
1359	451377139B	1377	151342140I	1342	691199800C	1409	100092142G
1427	691442145I	1442	440342035I	1459	240327800B	1392	701951141H

VIII. APPENDIX B: T.D.F. 40-80 PROGRAM FOR I.B.M. 650

A. Fourier Series Evaluation on a Grid Spacing of 1/40 or 1/80 of the Unit Cell

1. Function to be evaluated

The three dimensional Fourier series for the electron density is evaluated in the form

$$\begin{aligned}\rho(xyz) = \sum_{\ell=0}^{+\infty}\sum_{k=0}^{+\infty}\sum_{h=0}^{+\infty} \big[& A_1(hk\ell)\cos 2\pi hx \cos 2\pi ky \cos 2\pi\ell z \\ & + A_2(hk\ell)\sin 2\pi hx \sin 2\pi ky \cos 2\pi\ell z \\ & + A_3(hk\ell)\sin 2\pi hx \cos 2\pi ky \sin 2\pi\ell z \\ & + A_4(hk\ell)\cos 2\pi hx \sin 2\pi ky \sin 2\pi\ell z \\ & + B_1(hk\ell)\sin 2\pi hx \sin 2\pi ky \sin 2\pi\ell z \\ & + B_2(hk\ell)\cos 2\pi hx \cos 2\pi ky \sin 2\pi\ell z \\ & + B_3(hk\ell)\cos 2\pi hx \sin 2\pi ky \cos 2\pi\ell z \\ & + B_4(hk\ell)\sin 2\pi hx \cos 2\pi ky \cos 2\pi\ell z \big]\end{aligned}$$

where

$$\begin{aligned}A_1 &= A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\ A_2 &= -A'(hk\ell) - A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\ A_3 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) - A'(h\bar{k}\ell) + A'(\bar{h}k\ell) \\ A_4 &= -A'(hk\ell) + A'(\bar{h}\bar{k}\ell) + A'(h\bar{k}\ell) - A'(\bar{h}k\ell) \\ B_1 &= -B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\ B_2 &= B'(hk\ell) + B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\ B_3 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) - B'(h\bar{k}\ell) + B'(\bar{h}k\ell) \\ B_4 &= B'(hk\ell) - B'(\bar{h}\bar{k}\ell) + B'(h\bar{k}\ell) - B'(\bar{h}k\ell)\end{aligned}$$

and where A' and B' refer to the real and imaginary parts of the structure factor, multiplied by the appropriate multiplicity factor. For general structure factors, the factor is $\frac{2}{V}$. For structure factors having n zero indices, the factor is $\frac{2^{1-n}}{V}$. The special reflections are best handled by leaving out the required proportion of the coefficients.

The evaluation is carried out by successive one dimensional summations. The function is evaluated at intervals of either 1/80 or 1/40 of the unit cell. Two dimensional projections can be calculated by stopping after two summations.

2. Method of evaluation

The function is evaluated only over $x = 0, 1/4$, $y = 0, 1/4$ and $z = 0, 1/4$. The remainder of the cell is obtained by tabular expansion.

Trigonometric decks containing $\cos 2\pi hx$ and $\sin 2\pi hx$ for $h = 1, 2, \ldots, 39$ and $x = 1/80, 2/80, \ldots, 19/80$ (or, for the 1/40 case, $x = 1/40, 2/40, \ldots, 10/40$) are loaded onto the drum. The program forms the products and sums required for a one dimensional summation. The results may be punched in a format suitable for another summation or they may be punched in a format suitable for tabulation. If another summation is not required the results are punched out with 11 points per card. In the 1/80 case, two ranges are required. The first range contains the points 0/80, 1/80, ..., 10/80. The second range contains the points 11/80,...,20/80. It should be noted that the h,k and ℓ designations of the card fields are arbitrary but that the resultant x,y,z designations are defined in terms of the h,k,ℓ designations. It may be more efficient to change the h,k,ℓ designations in a particular problem.

Since the calculation is to be made with fixed decimal point, it may be necessary to use a scaling factor for the initial data. The coefficients are read onto the drum as xxxx.xxoooo. They are multiplied by 6 figure sin and cos (as .xxxxxxoooo). The upper accumulator is then stored. The last 4 digits of the product are carried during the summation but are dropped just before the punching operation. This leaves a maximum of 6 digits to be fed back for the next sum. The decimal point in the cards for tabulation is xxxx.xx. The extreme left hand digit should be 0. It is carried primarily as an overflow indication. The tabulator prints only xxx.xx.

3. <u>Method of expansion</u>

The expansion to the remainder of the unit cell is carried out on a Type 402 tabulator. The tabulation is based on the fact that $\left.\begin{matrix}\cos\\ \sin\end{matrix}\right\} 2\pi(hx + \frac{hn}{4})$ may be evaluated in terms of the values obtained in the first 1/4 x 1/4 x 1/4 block of the unit cell. This is shown in Table 15.

Table 15. Transformation of cos and sin by n/4

n	h even	h odd	h even	h odd
0	$\cos 2\pi hx$	$\cos 2\pi hx$	$\sin 2\pi hx$	$\sin 2\pi hx$
1	$\cos 2\pi hx'$[a]	$-\cos 2\pi hx'$[a]	$-\sin 2\pi hx'$[a]	$\sin 2\pi hx'$[a]
2	$\cos 2\pi hx$	$-\cos 2\pi hx$	$\sin 2\pi hx$	$-\sin 2\pi hx$
3	$\cos 2\pi hx'$[a]	$\cos 2\pi hx'$[a]	$-\sin 2\pi hx'$[a]	$-\sin 2\pi hx'$[a]

[a]Note that $x' = 1/4 - x$.

This expansion requires that the series be broken up into subseries during the I.B.M. 650 calculation. All terms of a given subseries must transform in the same way under a coordinate translation of n/4 in each direction (n = integer). In general the subseries must contain only terms having the same form of the trigonometric part and having the same evenness or oddness of each index. There are 64 possible subseries which can occur. If a completely general expansion is not required, it may be possible to combine certain subseries that transform similarly under the translations that are to be used. For a two dimensional summation, the maximum number of possible subseries is 8.

In order to generate these subseries, the detail cards must be sorted into subseries groups before a summation is carried out. They must also be sorted, within subseries groups, on the indices not being summed over.

Consequently, by changing the signs of the various subseries in the manner shown above, the summation on the 402 can generate the remaining 3/4 cycle in each direction from the results of the first 1/4 cycle. Note that, when $n = 2m+1$, the transformation $x' = 1/4 - x$ requires that the x' coordinate represent the lattice point. This means that the tabulated coordinates (from 0 to 1/4) must be translated and read in reverse.

The wiring changes required for the various blocks of the unit cell can be made by hand. However, in a full capacity Type 402, the various translations may be obtained by three, externally mounted, 4p4t rotary switches. The desired translations are then dialed on the switches. In conjunction with 4 pilot selectors, each switch determines the proper sign of one of the 3 factors that form the subseries. These 3 signs are then multiplied by the coselectors and used to control the counters for algebraic addition or subtraction. If it is desired, it can be so arranged that a heading card prints a code that designates the required switch setting and also tests the switch settings by printing, in the same code, the actual switch settings. The use of the heading card was found to be inconvenient in practice and no errors have resulted from not using this procedure.

4. Flow diagram, wiring information, and speed

The flow diagram for the T.D.F. 40-80 program is given in Figure 5. Zero indices are treated in a special manner in order to speed up the card reading rate.

The wiring diagrams for the I.B.M. 650 and 402 are given in Figures 6 and 7 respectively. The I.B.M. 650 wiring board uses storage entry C for input of detail cards, storage exit A for output of single coefficient cards, and storage exit C for output of multiple coefficient cards.

The detail cards will be read at a rate of approximately 100 cards per minute and the output cards will be punched at the maximum rate of 100 cards per minute. The internal calculations themselves require a negligible amount of time.

B. Operating Instructions

1. Card formats

The formats of the input detail cards at the various stages of the calculation are given in Table 16.

The formats of the multiple coefficient output cards at the various stages of the calculation are given in Table 17.

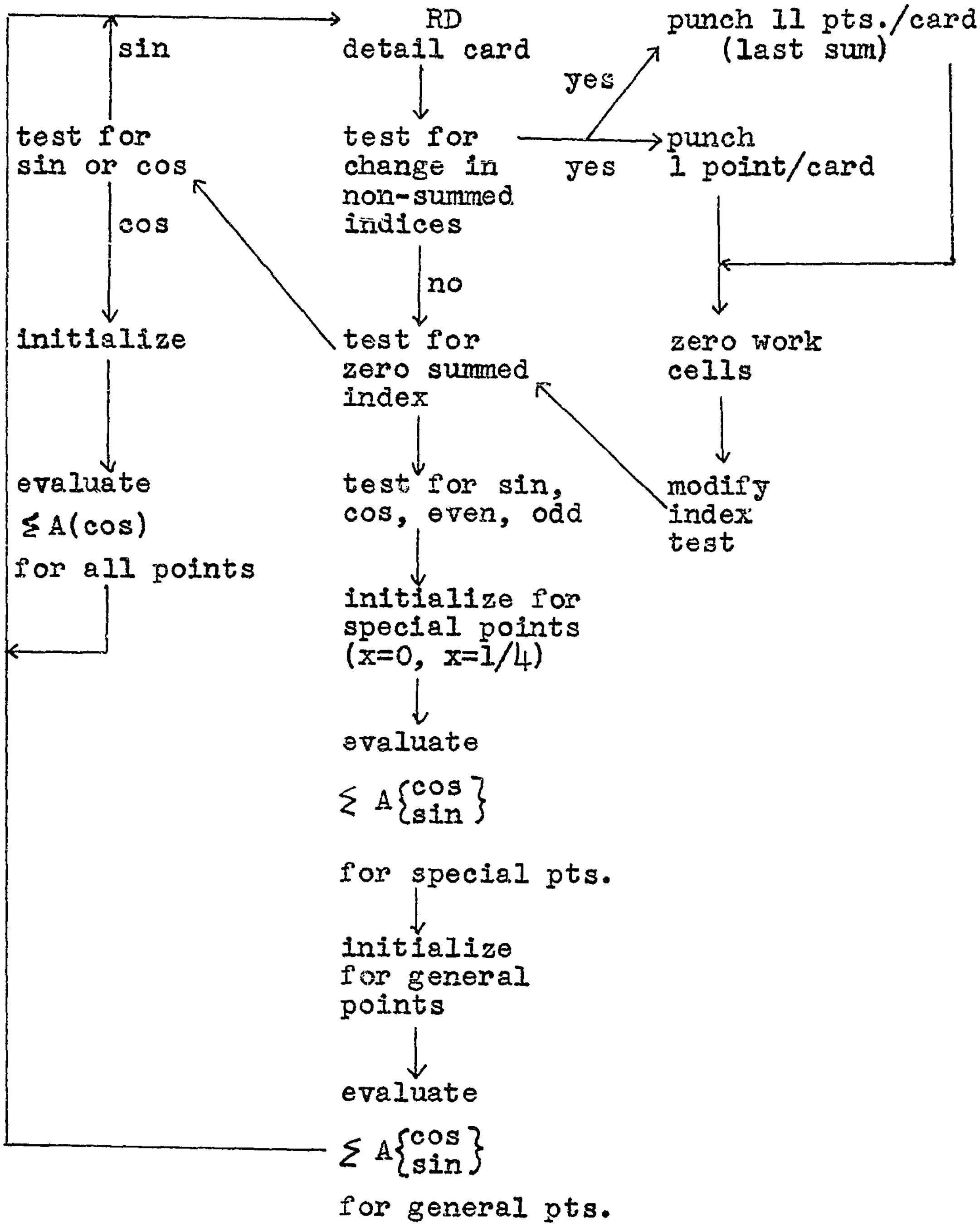
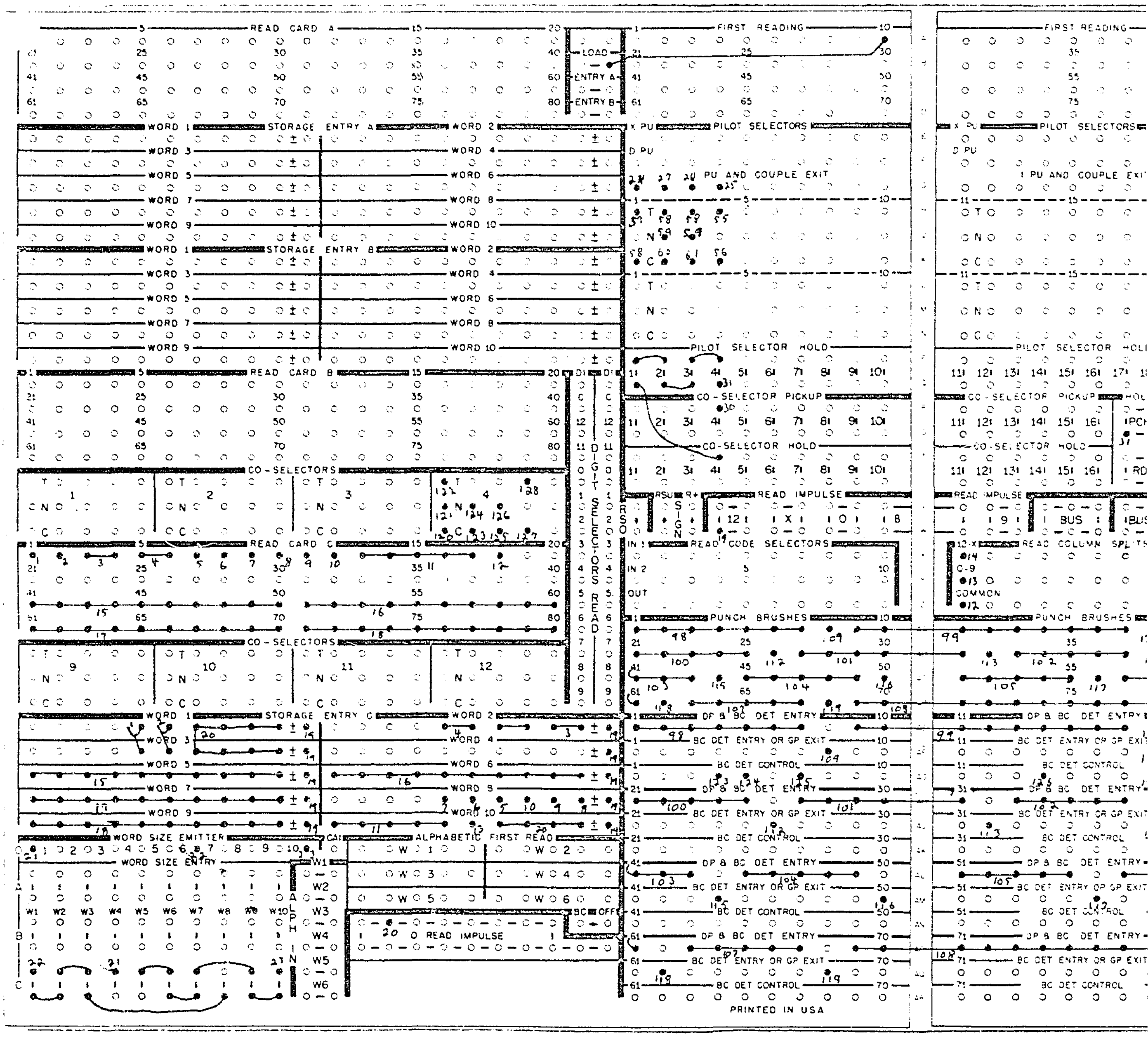
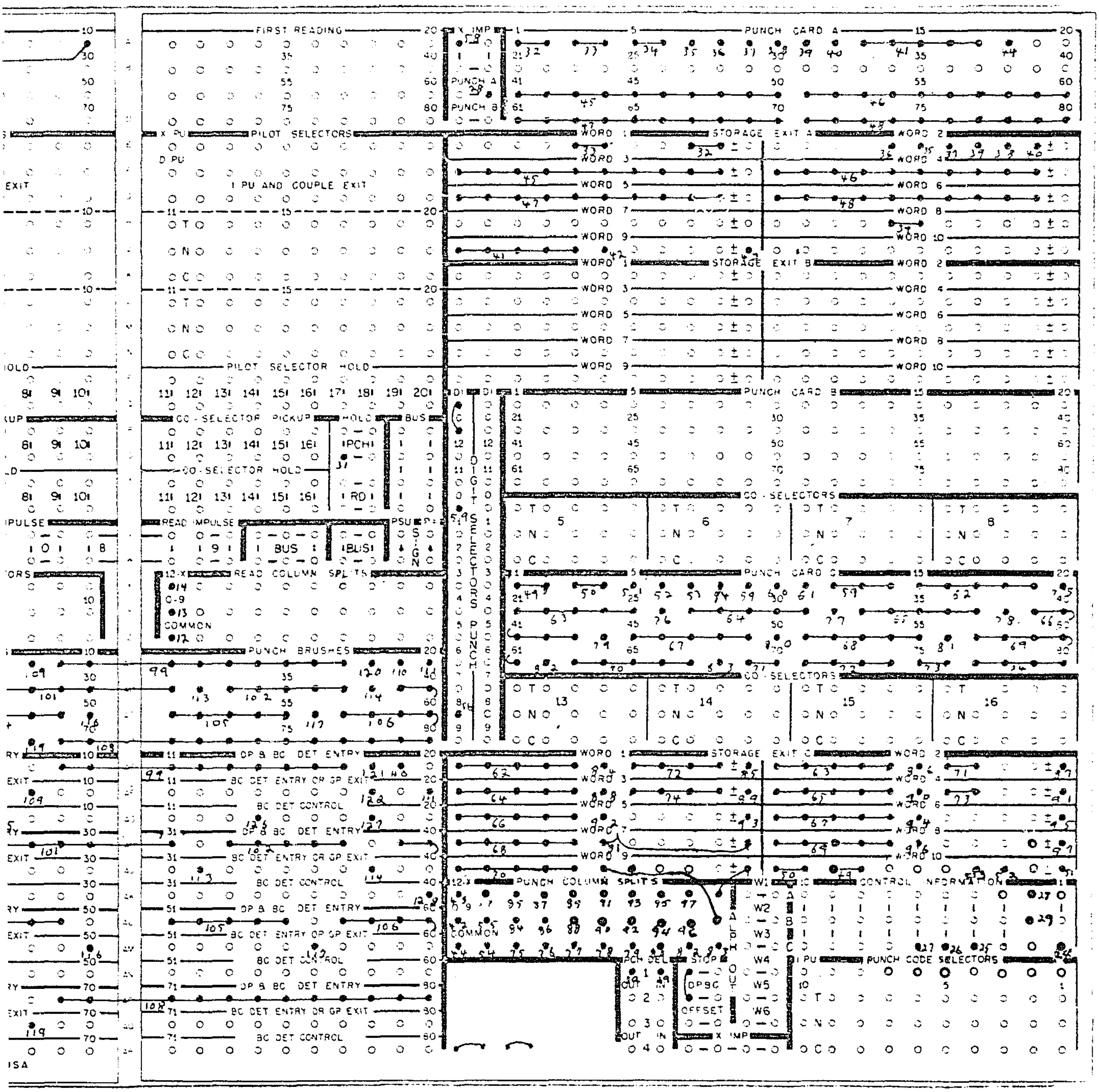


Figure 5. Flow diagram for T.D.F. 40-80

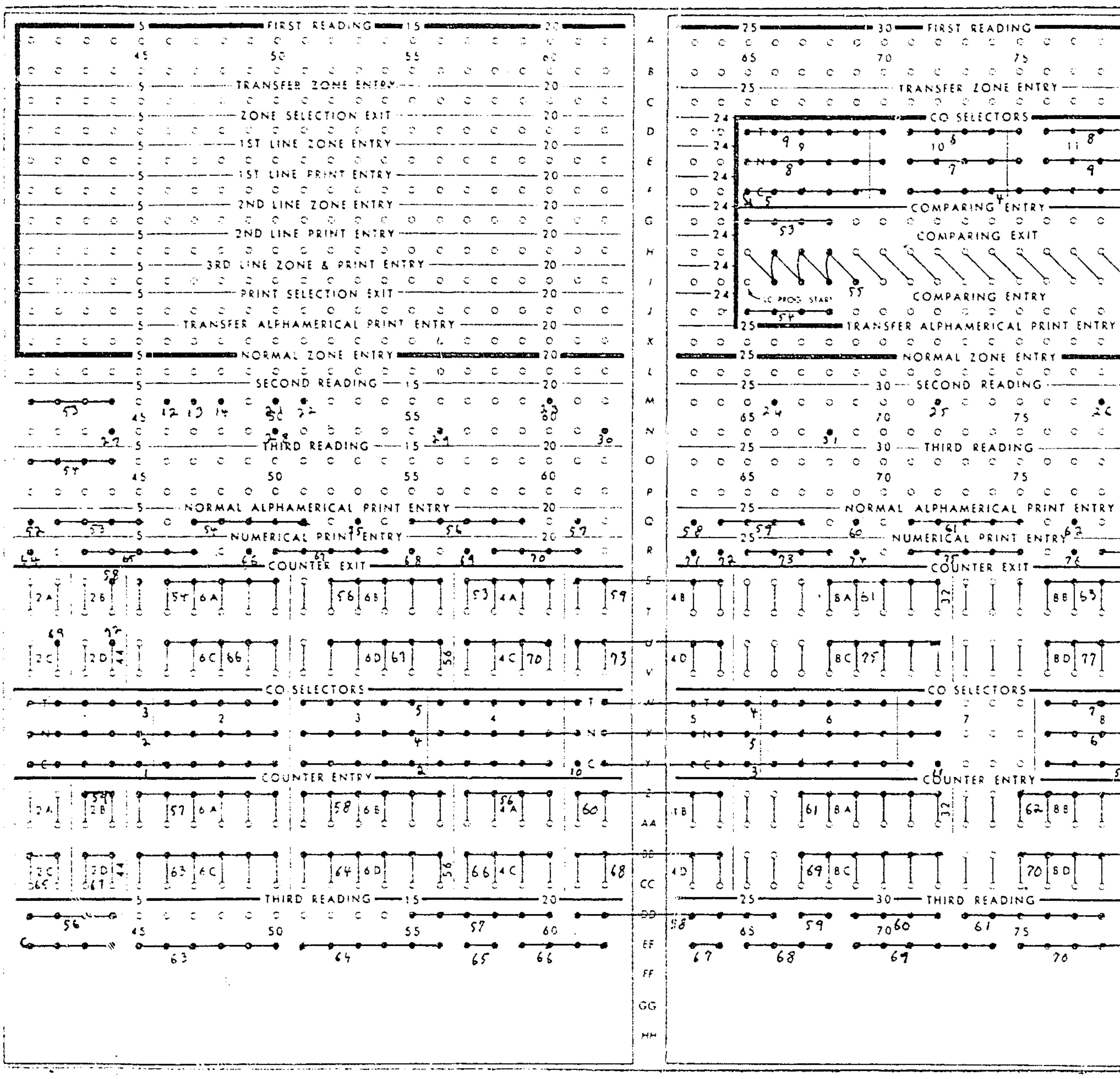
Figure 6. I.B.M. 650 plug board diagram for the T.D.F. 40-80 program


READ CARD A
FIRST READING
STORAGE ENTRY A
PILOT SELECTORS
PU AND COUPLE EXIT
STORAGE ENTRY B
PILOT SELECTOR HOLD
READ CARD B
CO-SELECTOR PICKUP
CO-SELECTOR HOLD
CO-SELECTORS
READ IMPULSE
READ CARD C
READ CODE SELECTORS
PUNCH BRUSHES
STORAGE ENTRY C
DP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
WORD SIZE EMITTER
ALPHABETIC FIRST READ
WORD SIZE ENTRY
READ IMPULSE
PRINTED IN USA



FIRST READING
PUNCH CARD A
PUNCH A
PUNCH B
X IMP
PILOT SELECTORS
I PU AND COUPLE EXIT
STORAGE EXIT A
STORAGE EXIT B
STORAGE EXIT C
PILOT SELECTOR HOLD
PUNCH CARD B
PUNCH CARD C
CO-SELECTOR PICKUP
CO-SELECTOR HOLD
CO-SELECTORS
READ IMPULSE
READ COLUMN SPLITS
PUNCH BRUSHES
DIGIT SELECTORS PUNCH
OP & BC DET ENTRY
BC DET ENTRY OR GP EXIT
BC DET CONTROL
PUNCH COLUMN SPLITS
CONTROL INFORMATION
PUNCH CODE SELECTORS
OFFSET
COMMON

Figure 7. I.B.M. 402 plug board diagram for the T.D.F. 40-80 program


FIRST READING
TRANSFER ZONE ENTRY
ZONE SELECTION EXIT
1ST LINE ZONE ENTRY
1ST LINE PRINT ENTRY
2ND LINE ZONE ENTRY
2ND LINE PRINT ENTRY
3RD LINE ZONE & PRINT ENTRY
PRINT SELECTION EXIT
TRANSFER ALPHAMERICAL PRINT ENTRY
NORMAL ZONE ENTRY
SECOND READING
THIRD READING
NORMAL ALPHAMERICAL PRINT ENTRY
NUMERICAL PRINT ENTRY
COUNTER EXIT
CO SELECTORS
COUNTER ENTRY
COMPARING ENTRY
COMPARING EXIT

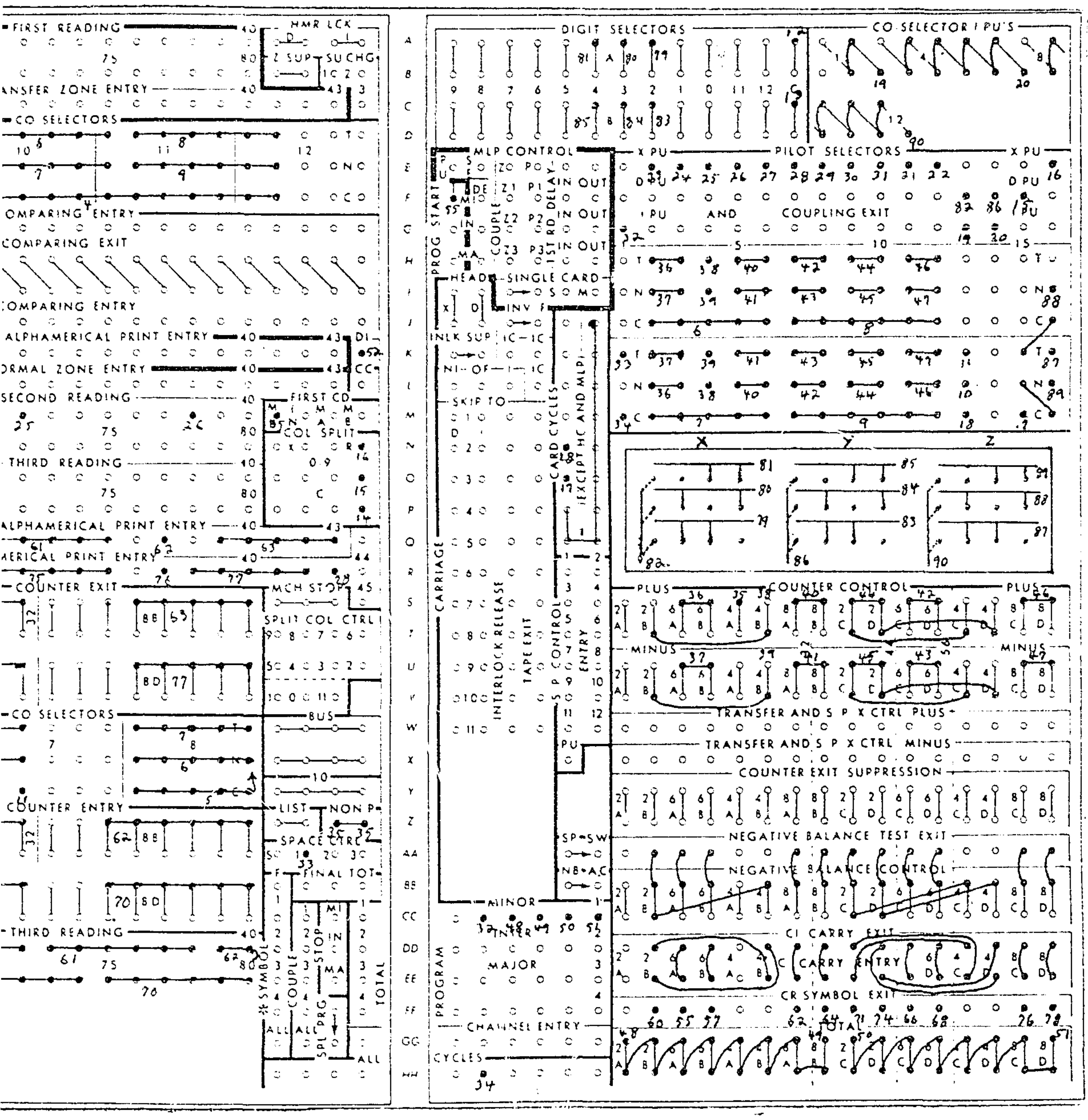

FIRST READING
HMR LCK
Z SUP
SUCHG
CO SELECTORS
COMPARING ENTRY
COMPARING EXIT
ALPHAMERICAL PRINT ENTRY
SECOND READING
FIRST CD
COL SPLIT
THIRD READING
COUNTER EXIT
MCH STOP
SPLIT COL CTRL
BUS
COUNTER ENTRY
LIST
NON P
SPACE CTRL
FINAL TOT
SYMBOL
COUPLE
SPL PRG
STOP
TOTAL
DIGIT SELECTORS
CO SELECTOR I PU'S
MLP CONTROL
PROG START
COUPLE
1ST RD DELAY
IN OUT
HEAD
SINGLE CARD
INV
INLK SUP
SKIP TO
CARD CYCLES
(EXCEPT HC AND MLP)
CARRIAGE
INTERLOCK RELEASE
TAPE EXIT
S P CONTROL
ENTRY
X PU
PILOT SELECTORS
D PU
I PU
AND
COUPLING EXIT
X
Y
Z
PLUS
COUNTER CONTROL
MINUS
TRANSFER AND S P X CTRL PLUS
TRANSFER AND S P X CTRL MINUS
COUNTER EXIT SUPPRESSION
SP-SW
NB-AC
NEGATIVE BALANCE TEST EXIT
NEGATIVE BALANCE CONTROL
MINOR
MAJOR
PROGRAM
CI CARRY EXIT
CARRY ENTRY
CR SYMBOL EXIT
CHANNEL ENTRY
CYCLES

Table 16. Input detail cards and single coefficient output cards

Card col.	Contents 1st sum	2nd sum	3rd sum	Comments
1-2	h	k	ℓ	Summation occurs over the index in col. 1-2
3-4	k	ℓ	x	
5-6	ℓ	x	y	
7	α_h	α_k	α	α_i = 8 if i is even
8	α_k	α	α_h	α_i = 9 if i is odd
9	α_ℓ	α_h	α_k	
10	β_h	β_k	β_ℓ	
11	β_k	β_ℓ	β_h	β_j = 8 if cos $2\pi jx$
12	β_ℓ	β_h	β_k	β_j = 9 if sin $2\pi jx$
13-18	Fourier coef A; xxxx.xx			Sign is overpunched in col. 18
41-50	10 1009 1030			x = -.
51-60	69 0959 1031			These orders are used in the program. They must be punched into the first sum detail cards only if multiple coefficient cards are to be punched.
61-70	23 0977 1343			
71-80	65 0000 1010			

Table 17. Multiple coefficient output cards

Card col.	Contents 2nd sum	3rd sum	Comments
1-2	ℓ	x	x switch expands col. 1-2 y switch expands col. 3-4 z switch expands card line
3-4	x	y	
5	x or no x	x or no x	no x first range x second range
6	C_ℓ	C_h	C = 1 for E.C. 2 for O.C. C = 3 for E.S. 4 for O.S. D = blank for O.S. 8 for E.S. D = x for O.C. x/8 for E.C.
7	C_h	C_k	
8	D_k	D_ℓ	
10	sign of value in 69-74		
11	sign of value in 75-80		
15-20	y = 0,11	z = 0,11	
21-26	y = 1,12	z = 1,12	
.	.	.	
.	.	.	The second value is for the second range
.	.	.	
.	.	.	
69-74	y = 9,20	z = 9,20	
75-80	y = 10,-	z = 10,-	

2. <u>Assembly of program deck</u>

To place the program in operation, set the console switches for normal operation with error switches set to stop. The storage entry switches are set at 70 0004 xxxx.

Computer reset and program start will start the loading of the program deck and detail cards. The program deck is made up in the following order:

(a) Drum clear and four-order load routine, (This consists of five load cards which must be kept in order.),

(b) Program deck, (This deck also contains the orders for single point punching and 1/80 interval. These are four-order type load cards.),

(c) Sine and cosine decks for the desired interval, (These are four-order type load cards.),

(d) Calculate by 1/40 (one control card), (This is four-order type load card and is used only if 1/40 intervals are desired.),

(e) Transfer card, (This card transfers to the read instruction at 0050 of 70 0951 0048.),

(f) Modification cards for type of punching desired,

(g) Detail cards, (The input detail cards must be sorted on constant indices and then be sorted into subseries.),

(h) Last card, (The program punches on a change of index. The last card furnishes such a change so that the last set of sums may be punched. It corresponds to a detail card with zero indices and calls for a sin sin sin product. This leaves the work cells set at zero. The program register will contain the RD instruction at 0300 RD 70 0951 0098.).

In order to rerun for the next sum the storage entry switches should be reset to 00 0000 0050. Pressing computer reset will transfer control to the read instruction at 0050.

The cards in items f, g and h are then run through the machine. The cards in items a, b, c, d and e are used only to put the program on the drum.

3. Tabulation

The final output cards are sorted on columns 4 through 1 and then sorted into two ranges by sorting on column 5. These cards are then tabulated. The tabulator sheet of paper is printed in the same format no matter what the setting of the three translation switches may be. At the left hand side, the contents of columns 1-4 are printed. The third coordinate of the point is implied in the position of the column containing the value of the Fourier series for that point. These columns are labeled, from left to right, by 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 for the first range. The second range results are tabulated below the first range results. The columns in the second range are labeled, from left to right, by 11, 12, 13, 14, 15, 16, 17, 18, 19, 20. The coordinates for points using various translations are obtained in the manner previously discussed.

4. Empty drum cells

The following locations are not used in this program:

1950	1995	1648
0896	1348	1698
0946	1398	1748
1795	1448	1798

1845	1498	1848
1895	1548	1898
1945	1598	1948
		1998.

5. Control card formats

The drum zero card and the four-order loading routine are given in Table 18.

A card punched with

69 0952 0953 45 1444 0954 24 1150 0950 69 0955 0956
45 1444 0048 24 1150 0050 00 0000 0000 00 0000 0000

in columns 1 through 80 will zero the work cells used in storing intermediate sums. This card is not used in ordinary operation.

The calculate by 1/40 control card is a load card punched from column 1 to 80 with

24 1490 1645 20 1496 0300 24 1017 1695 00 0000 1034
24 0490 1745 21 1496 0300 24 0491 0985 21 1497 0300 .

The various punch control cards for multiple coefficient output are listed below.

(a) Punch two ranges and both even and odd index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 1195 0955
24 1942 0956 69 1245 0957 24 1992 0050 00 0000 0000

(b) Punch two ranges and only even index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 1195 0955

24 1942 0956 69 1295 0957 24 1992 0050 00 0000 0000

(c) Punch one range and both even and odd index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 0955 0956

71 0977 0650 24 1942 0050 00 0000 0000 00 0000 0000

(d) Punch one range and only even index results.

69 0952 0953 44 1200 0149 24 0973 0954 69 0955 0956

71 0977 0796 24 1942 0050 00 0000 0000 00 0000 0000

(e) Punch single coefficient cards. These are used if it is desired to return to single coefficient output after switching to multiple coefficient output has been used. There are three cards required.

Card 1 is

69 0952 0953 44 0194 0149 24 0973 0954 69 0955 0956

10 1009 1030 24 0979 0050 00 0000 0000 00 0000 0000 .

Card 2 is

69 0952 0953 69 0959 1031 24 0980 0954 69 0955 0956

23 0977 1343 24 0981 0050 00 0000 0000 00 0000 0000 .

Card 3 is

69 0952 0953 65 0000 1010 24 0982 0050 00 0000 0000

00 0000 0000 00 0000 0000 00 0000 0000 00 0000 0000 .

The transfer from four-order load routine card is a non-load card punched with a zero in each column.

Table 18. Drum zero and four-order load routine

Field	Operation code	Address Data	Address Instruction	Remarks
1	00	0001	0000	
2	00	0000	0000	
3	10	0001	8003	
4	61	0008	0007	drum zero
5	24	0000	8003	
6	70	0004	0004	(1)
7	69	0006	0005	
8	20	1999	0003	
1	69	0002	0003	
2	69	0952	0951	load load routine
3	24	1595	0000	
4	69	0005	0006	
5	70	0984	0050	(2)
6	24	0985	0001	
7	00	0000	0000	
8	00	0000	0000	
1	69	0002	0003	
2	69	0956	0955	
3	24	1695	0000	
4	69	0005	0006	(3)
5	69	0954	0953	
6	24	1645	0001	
7	00	0000	0000	
8	00	0000	0000	
1	69	0002	0003	
2	65	0951	1545	
3	24	0984	0000	
4	69	0005	0006	(4)
5	69	0958	0957	
6	24	1745	0001	
7	00	0000	0000	
8	00	0000	0000	
1	00	0000	0000	
2	00	0000	0000	
3	00	0000	0000	(5)
4	69	0005	0006	
5	45	1595	0952	
6	24	0984	0985	
7	00	0000	0000	
8	00	0000	0000	

6. <u>The program deck</u>

The cards in the program deck are listed in Table 19 with the contents of each card displayed on one line. The trigonometric decks for 1/40 interval are listed in Table 20. The 1/80 interval decks are listed in Table 21. These addresses and orders must be made into four-order load cards.

TABLE 19. PROGRAM ORDERS FOR T.D.F. 40-80 (SYMBOLS
* AND ¤ REPRESENT X/0 AND Y/0)

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0194690247020¤	0247000000008¤	0200240986080¤	0800650978189C
1893940596029H	0298160444059F	0444000000100¤	0596200978049D
0494690047085¤	0047440348094I	0850241044054D	0544650447090¤
0447100996049E	0900210984059D	0594118001800B	0495440899134E
0899460644084D	0644110497069D	0497000000000A	0694210985074D
0744118001079D	0794100497054E	0844210985089D	0894118001054E
0545710977094D	0944100984099D	0994110547104D	0547000020000¤
0348108001039H	0398100645099I	0999151094090¤	1094000050000¤
0949691144059G	1144440348095¤	0597241044064G	0647650978119D
1194150697124D	0697000000100¤	1244200978129D	1294650747090¤
0747100997049E	0950651344800B	1344210996100¤	1000161943079G
1943211996100¤	0797451050139D	1050151993800B	1993212046100¤
1394650847800B	0847210997110¤	1100161494115¤	1494211997110¤
1444150897800B	0897212047110¤	1200650977144B	1442698003024H
0248230954149B	1492300002034I	0349158001154B	1542350006159B
1592150978159D	1642940399029G	0297160245039I	0245000000100¤
0399200986059E	0595691544039G	1544230978040¤	0397240350034G
0347650550103B	0550690996800C	1032101036800B	1036240977099A
0991110044044I	0044240985099A	0449440955144E	1009240986099A
1030151035800B	1035000050000¤	1031221037800A	1010690977169C
1693300004095G	1343300004139C	1393350002049I	0499461742179B
1742160295054I	0295000000000H	1792150345054I	0345000000000I
0549690978035¤	0400651037009F	0096150599800B	0599000050003H
1048690979144C	1443300004014F	0146230979149C	1493300004154C
1543350002064I	0649461842189B	1842160295069I	1892150345069I
0699690980024F	0246230980189D	0600660986029F	0296200986159C
1593690346074I	0346230978169B	0749240350164C	1643650396024D
0396000550000¤	0244150550103B	1692658003079I	0799690979029D
0294230979034D	0344690980039D	0394230980094H	0650670986174C
0446151500074F	1500000000100¤	0849200986179C	1793690496039E
0496230978040¤	0395240350184C	1843650546044E	0546690997800C
0445200550103B	0050700951004H	0300700951009H	0971210977009E
0095690958096I	0969240978014I	0098600952096E	0965110968097C
0973440194014I	0149600951100E	1005690958101A	1011450964004F
0046910099030¤	0099650960096F	0966201025098G	0987150996097D
0974200996104I	1049651025104A	1041151046104¤	1040201046109I
1099651025109A	1091151096109¤	1090201096114I	1149651025114A
1141151146114¤	1140201146119I	1199651025119A	1191151196119¤
1190201196124I	1249651025124A	1241151246124¤	1240201246129I
1299651025129A	1291151296129¤	1290201296134I	1349651025134A
1341151346134¤	1340201346139I	1399651025139A	1391151396139¤
1390201396144I	1449651025144A	1441151446144¤	1440201446149I
1499651025149A	1491151496149¤	1490201496154I	1549651025154A
1541151546154¤	1540201546159I	1599651025159A	1591151596159¤

TABLE 19. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1590201596164I	1649651025164A	1641151646164⌑	1640201646169I
1699651025169A	1691151696169⌑	1690201696174I	1749651025174A
1741151746174⌑	1740201746179I	1799651025179A	1791151796179⌑
1790201796184I	1849651025184A	1841151846184⌑	1840201846189I
1899651025189A	1891151896189⌑	1890201896194I	1949651025194A
1941151946194⌑	1940201946199I	1999651025199A	1991151996199⌑
1990201996030⌑	0964910967101I	0967941020102B	1020668003102G
1027150094019I	0094190040004B	0199201015097F	0976201037109C
1093650996100B	1002150960103I	1039200996029I	0299600951100F
1006100963101G	0963000001000⌑	1022668003099⌑	0990150993009G
0993190040004C	0097201015097E	0975201037014D	0144650997100C
1003150960098H	0988200997015⌑	0150600953100H	1008100963101G
1019941023102F	1023668003098I	0989151043019H	1043191090004B
0198201015102D	1024201037014G	0147600951101G	1026668003104B
1042150145024I	0145191090004C	0249201015102A	1021201037019G
0197600951101G	1017191028101C	1028000000002E	1013300002102I
1029691033103H	1033000000000⌑	1038231092019E	0195658001100D
1004300001800B	0000000000103D	0500000000103D	0250690958101F
0750690958101H	1016941143119C	1018941243129C	1143651996114B
1193651997119B	1243651996124B	1293651997129B	1142150960134B
1192150960139B	1242160960134B	1292160960139B	1342201996103D
1392201997103D	1034651037099B	0992150045004I	0045000050005⌑
0049200954100G	1007600960101E	0092101096009⌑	0142101146014⌑
0192101196019⌑	0242101246024⌑	0292101296029⌑	0342101346034⌑
0392101396039⌑	0442101446044⌑	0492101496049⌑	0542101546054⌑
0592101596059⌑	0642101646064⌑	0692101696069⌑	0742101746074⌑
0792101796079⌑	0842101846084⌑	0892101896089⌑	0942101946094⌑
0043101047004A	0093101097009A	0143101147014A	0193101197019A
0243101247024A	0293101297029A	0343101347034A	0393101397039A
0443101447044A	0493101497049A	0543101547054A	0593101597059A
0643101647064A	0693101697069A	0743101747074A	0793101797079A
0843101847084A	0893101897089A	0943101947094A	0940211946030⌑
0041211047100A	0091211097100A	0141211147100A	0191211197100A
0641211647100A	0691211697100A	0741211747100A	0791211797100A
0441211447100A	0491211497100A	0541211547100A	0591211597100A
0241211247100A	0291211297100A	0341211347100A	0391211397100A
0841211847100A	0891211897100A	0941211947030⌑	0645000001000⌑
1594920947125⌑	0947951644049H	1644160448130⌑	0448000008007⌑
0498160695130⌑	0695000009006⌑	1250951694054H	1694160598130⌑
0598000008006⌑	0745000009005⌑	1300698002174D	1744930148135⌑
0148961794019F	1794160648101B	0648000080070⌑	0196161400101B
1350961844064F	1400000090060⌑	1844160698101B	0698000080060⌑
0646161450101B	1450000090050⌑	1894910748155⌑	0748650986079E
0948650978104E	1045910998170⌑	0998650986194D	1944961992175⌑
0945000080000⌑	1600150995165⌑	0995000090000⌑	1650200986194B

TABLE 19. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0848000009000¤	0696690978089E	0895910898160¤	0898150945165¤
0795150798069F	0798000008000¤	1550650986084E	0845150848069F
1750151098199B	1098000010000¤	1700650986109E	1095961148149E
1148161098149E	0746698002199D	1994961198180¤	1198160945185¤
1800160995185¤	1850698002114E	1145951248190¤	1248160798084I
1900160848084I	1012698002164B	1150451444004H	0048600952096B
0962210968097A	0042101046004¤	1001650954096A	0961201015097B
0972201037099B	0040211046100A	0090211096100A	0140211146100A
0190211196100A	0240211246100A	0290211296100A	0340211346100A
0390211396100A	0440211446100A	0490211496100A	0540211546100A
0590211596100A	0640211646100A	0690211696100A	0740211746100A
0790211796100A	0840211846100A	0890211896100A	0796690970084F
0548160745130¤	1743940446079F	0846240550095¤	0970690996800C
0978000088888H	0979101009103¤	0980690959103A	0981230977134C
0982650000101¤	1495200986199B	1345461395094D	1395100497094D
1195710977060¤	1245710977065¤	1295710977079F	1298000050000¤
1445151298095F	1245710977065¤	1295710977079F	1298000050000¤
1750151098149E	1495200986199B		

TABLE 20. SINE AND COSINE TABLE BY 1/40 INTERVAL (SYMBOLS * AND ⌑ REPRESENT X/0 AND Y/0)

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1051156434000*	1052309017000*	1053453990000*	1054587785000*
1055707107000*	1056809017000*	1057891007000*	1058951057000*
1059987688000*	1060999999000*	1061987688000*	1062951057000*
1063891007000*	1064809017000*	1065707107000*	1066587785000*
1067453990000*	1068309017000*	1069156434000*	1070000000000*
1071156434000⌑	1072309017000⌑	1073453990000⌑	1074587785000⌑
1075707107000⌑	1076809017000⌑	1077891007000⌑	1078951057000⌑
1079987688000⌑	1080999999000⌑	1081987688000⌑	1082951057000⌑
1083891007000⌑	1084809017000⌑	1085707107000⌑	1086587785000⌑
1087453990000⌑	1088309017000⌑	1089156434000⌑	1101309017000*
1102587785000*	1103809017000*	1104951057000*	1105999999000*
1106951057000*	1107809017000*	1108587785000*	1109309017000*
1110000000000*	1111309017000⌑	1112587785000⌑	1113809017000⌑
1114951057000⌑	1115999999000⌑	1116951057000⌑	1117809017000⌑
1118587785000⌑	1119309017000⌑	1120000000000⌑	1121309017000*
1122587785000*	1123809017000*	1124951057000*	1125999999000*
1126951057000*	1127809017000*	1128587785000*	1129309017000*
1130000000000*	1131309017000⌑	1132587785000⌑	1133809017000⌑
1134951057000⌑	1135999999000⌑	1136951057000⌑	1137809017000⌑
1138587785000⌑	1139309017000⌑	1151453990000*	1152809017000*
1153987688000*	1154951057000*	1155707107000*	1156309017000*
1157156434000⌑	1158587785000⌑	1159891007000⌑	1160999999000⌑
1161891007000⌑	1162587785000⌑	1163156434000⌑	1164309017000*
1165707107000*	1166951057000*	1167987688000*	1168809017000*
1169453990000*	1170000000000*	1171453990000⌑	1172809017000⌑
1173987688000⌑	1174951057000⌑	1175707107000⌑	1176309017000⌑
1177156434000*	1178587785000*	1179891007000*	1180999999000*
1181891007000*	1182587785000*	1183156434000*	1184309017000⌑
1185707107000⌑	1186951057000⌑	1187987688000⌑	1188809017000⌑
1189453990000⌑	1201587785000*	1202951057000*	1203951057000*
1204587785000*	1205000000000*	1206587785000⌑	1207951057000⌑
1208951057000⌑	1209587785000⌑	1210000000000⌑	1211587785000*
1212951057000*	1213951057000*	1214587785000*	1215000000000*
1216587785000⌑	1217951057000⌑	1218951057000⌑	1219587785000⌑
1220000000000⌑	1221587785000*	1222951057000*	1223951057000*
1224587785000*	1225000000000*	1226587785000⌑	1227951057000⌑
1228951057000⌑	1229587785000⌑	1230000000000⌑	1231587785000*
1232951057000*	1233951057000*	1234587785000*	1235000000000*
1236587785000⌑	1237951057000⌑	1238951057000⌑	1239587785000⌑
1251707107000*	1252999999000*	1253707107000*	1254000000000*
1255707107000⌑	1256999999000⌑	1257707107000⌑	1258000000000⌑
1259707107000*	1260999999000*	1261707107000*	1262000000000*
1263707107000⌑	1264999999000⌑	1265707107000⌑	1266000000000⌑
1267707107000*	1268999999000*	1269707107000*	1270000000000*

TABLE 20. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
1271	707107000□	1272	999999000□	1273	707107000□	1274	000000000□
1275	707107000*	1276	999999000*	1277	707107000*	1278	000000000*
1279	707107000□	1280	999999000□	1281	707107000□	1282	000000000□
1283	707107000*	1284	999999000*	1285	707107000*	1286	000000000*
1287	707107000□	1288	999999000□	1289	707107000□	1301	809017000*
1302	951057000*	1303	309017000*	1304	587785000□	1305	999999000□
1306	587785000□	1307	309017000*	1308	951057000*	1309	809017000*
1310	000000000*	1311	809017000□	1312	951057000□	1313	309017000□
1314	587785000*	1315	999999000*	1316	587785000*	1317	309017000□
1318	951057000□	1319	809017000□	1320	000000000□	1321	809017000*
1322	951057000*	1323	309017000*	1324	587785000□	1325	999999000□
1326	587785000□	1327	309017000*	1328	951057000*	1329	809017000*
1330	000000000*	1331	809017000□	1332	951057000□	1333	309017000□
1334	587785000*	1335	999999000*	1336	587785000*	1337	309017000□
1338	951057000□	1339	809017000□	1351	891007000*	1352	809017000*
1353	156434000□	1354	951057000□	1355	707107000□	1356	309017000*
1357	987688000*	1358	587785000*	1359	453990000□	1360	999999000□
1361	453990000□	1362	587785000*	1363	987688000*	1364	309017000*
1365	707107000□	1366	951057000□	1367	156434000□	1368	809017000*
1369	891007000*	1370	000000000*	1371	891007000□	1372	809017000□
1373	156434000*	1374	951057000*	1375	707107000*	1376	309017000□
1377	987688000□	1378	587785000□	1379	453990000*	1380	999999000*
1381	453990000*	1382	587785000□	1383	987688000□	1384	309017000□
1385	707107000*	1386	951057000*	1387	156434000*	1388	809017000□
1389	891007000□	1401	951057000*	1402	587785000*	1403	587785000□
1404	951057000□	1405	000000000□	1406	951057000*	1407	587785000*
1408	587785000□	1409	951057000□	1410	000000000□	1411	951057000*
1412	587785000*	1413	587785000□	1414	951057000□	1415	000000000□
1416	951057000*	1417	587785000*	1418	587785000□	1419	951057000□
1420	000000000□	1421	951057000*	1422	587785000*	1423	587785000□
1424	951057000□	1425	000000000□	1426	951057000*	1427	587785000*
1428	587785000□	1429	951057000□	1430	000000000□	1431	951057000*
1432	587785000*	1433	587785000□	1434	951057000□	1435	000000000□
1436	951057000*	1437	587785000*	1438	587785000□	1439	951057000□
1451	987688000*	1452	309017000*	1453	891007000□	1454	587785000□
1455	707107000*	1456	809017000*	1457	453990000□	1458	951057000□
1459	156434000*	1460	999999000*	1461	156434000*	1462	951057000□
1463	453990000□	1464	809017000*	1465	707107000*	1466	587785000□
1467	891007000□	1468	309017000*	1469	987688000*	1470	000000000*
1471	987688000□	1472	309017000□	1473	891007000*	1474	587785000*
1475	707107000□	1476	809017000□	1477	453990000*	1478	951057000*
1479	156434000□	1480	999999000□	1481	156434000□	1482	951057000*
1483	453990000*	1484	809017000□	1485	707107000□	1486	587785000*
1487	891007000*	1488	309017000□	1489	987688000□	1501	999999000*
1502	000000000*	1503	999999000□	1504	000000000□	1505	999999000*

TABLE 20. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1506000000000*	1507999999000□	1508000000000□	1509999999000*
1510000000000*	1511999999000□	1512000000000□	1513999999000*
1514000000000*	1515999999000□	1516000000000□	1517999999000*
1518000000000*	1519999999000□	1520000000000□	1521999999000*
1522000000000*	1523999999000□	1524000000000□	1525999999000*
1526000000000*	1527999999000□	1528000000000□	1529999999000*
1530000000000*	1531999999000□	1532000000000□	1533999999000*
1534000000000*	1535999999000□	1536000000000□	1537999999000*
1538000000000*	1539999999000□	1536000000000□	1537999999000*
0001987688000□	0002951057000□	0003891007000□	0004809017000□
0005707107000□	0006587785000□	0007453990000□	0008309017000□
0009156434000□	0010000000000□	0011156434000*	0012309017000*
0013453990000*	0014587785000*	0015707107000*	0016809017000*
0017891007000*	0018951057000*	0019987688000*	0020999999000*
0021987688000*	0022951057000*	0023891007000*	0024809017000*
0025707107000*	0026587785000*	0027453990000*	0028309017000*
0029156434000*	0030000000000*	0031156434000□	0032309017000□
0033453990000□	0034587785000□	0035707107000□	0036809017000□
0037891007000□	0038951057000□	0039987688000□	0051951057000□
0052809017000□	0053587785000□	0054309017000□	0055000000000□
0056309017000*	0057587785000*	0058809017000*	0059951057000*
0060999999000*	0061951057000*	0062809017000*	0063587785000*
0064309017000*	0065000000000*	0066309017000□	0067587785000□
0068809017000□	0078809017000*	0069951057000□	0070999999000□
0071951057000□	0072809017000□	0073587785000□	0074309017000□
0075000000000□	0076309017000*	0077587785000*	0079951057000*
0080999999000*	0081951057000*	0082809017000*	0083587785000*
0084309017000*	0085000000000*	0086309017000□	0087587785000□
0088809017000□	0089951057000□	0101891007000□	0102587785000□
0103156434000□	0104309017000*	0105707107000*	0106951057000*
0107987688000*	0108809017000*	0109453990000*	0110000000000*
0111453990000□	0112809017000□	0113987688000□	0114951057000□
0115707107000□	0116309017000□	0117156434000*	0118587785000*
0119891007000*	0120999999000*	0121891007000*	0122587785000*
0123156434000*	0124309017000□	0125707107000□	0126951057000□
0127987688000□	0128809017000□	0129453990000□	0130000000000□
0131453990000*	0132809017000*	0133987688000*	0134951057000*
0135707107000*	0136309017000*	0137156434000□	0138587785000□
0139891007000□	0151809017000□	0152309017000□	0153309017000*
0154809017000*	0155999999000*	0156809017000*	0157309017000*
0158309017000□	0159809017000□	0160999999000□	0161809017000□
0162309017000□	0163309017000*	0164809017000*	0165999999000*
0166809017000*	0167309017000*	0168309017000□	0169809017000□
0170999999000□	0171809017000□	0172309017000□	0173309017000*
0174809017000*	0175999999000*	0176809017000*	0177309017000*

TABLE 20. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0178309017000⌑	0179809017000⌑	0180999999000⌑	0181809017000⌑
0182309017000⌑	0183309017000*	0184809017000*	0185999999000*
0186809017000*	0187309017000*	0188309017000⌑	0189809017000⌑
0201707107000⌑	0202000000000⌑	0203707107000*	0204999999000*
0205707107000*	0206000000000*	0207707107000⌑	0208999999000⌑
0209707107000⌑	0210000000000⌑	0211707107000*	0212999999000*
0213707107000*	0214000000000*	0215707107000⌑	0216999999000⌑
0217707107000⌑	0218000000000⌑	0219707107000*	0220999999000*
0221707107000*	0222000000000*	0223707107000⌑	0224999999000⌑
0225707107000⌑	0226000000000⌑	0227707107000*	0228999999000*
0229707107000*	0230000000000*	0231707107000⌑	0232999999000⌑
0233707107000⌑	0234000000000⌑	0235707107000*	0236999999000*
0237707107000*	0238000000000*	0239707107000⌑	0251587785000⌑
0252309017000*	0253951057000*	0254809017000*	0255000000000*
0256809017000⌑	0257951057000⌑	0258309017000⌑	0259587785000*
0260999999000*	0261587785000*	0262309017000⌑	0263951057000⌑
0264809017000⌑	0265000000000⌑	0266809017000*	0267951057000*
0268309017000*	0269587785000⌑	0270999999000⌑	0271587785000⌑
0272309017000*	0273951057000*	0274809017000*	0275000000000*
0276809017000⌑	0277951057000⌑	0278309017000⌑	0279587785000*
0280999999000*	0281587785000*	0282309017000⌑	0283951057000⌑
0284809017000⌑	0285000000000⌑	0286809017000*	0287951057000*
0288309017000*	0289587785000⌑	0301453990000⌑	0302587785000*
0303987688000*	0304309017000*	0305707107000⌑	0306951057000⌑
0307156434000⌑	0308809017000*	0309891007000*	0310000000000*
0311891007000⌑	0312809017000⌑	0313156434000*	0314951057000*
0315707107000*	0316309017000⌑	0317987688000⌑	0318587785000⌑
0319453990000*	0320999999000*	0321453990000*	0322587785000⌑
0323987688000⌑	0324309017000⌑	0325707107000*	0326951057000*
0327156434000*	0328809017000⌑	0329891007000⌑	0330000000000⌑
0331891007000*	0332809017000*	0333156434000⌑	0334951057000⌑
0335707107000⌑	0336309017000*	0337987688000*	0338587785000*
0339453990000⌑	0351309017000⌑	0352809017000*	0353809017000*
0354309017000⌑	0355999999000⌑	0356309017000⌑	0357809017000*
0358809017000*	0359309017000⌑	0360999999000⌑	0361309017000⌑
0362809017000*	0363809017000*	0364309017000⌑	0365999999000⌑
0366309017000⌑	0367809017000*	0369309017000⌑	0370999999000⌑
0371309017000⌑	0372809017000*	0373809017000*	0374309017000⌑
0375999999000⌑	0376309017000⌑	0377809017000*	0368809017000*
0378809017000*	0379309017000⌑	0380999999000⌑	0381309017000⌑
0382809017000*	0383809017000*	0384309017000⌑	0385999999000⌑
0386309017000⌑	0387809017000*	0388809017000*	0389309017000⌑
0401156434000⌑	0402951057000*	0403453990000*	0404809017000⌑
0405707107000⌑	0406587785000*	0407891007000*	0408309017000⌑
0409987688000⌑	0410000000000⌑	0411987688000*	0412309017000*

TABLE 20. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0413891007000□	0414587785000□	0415707107000*	0416809017000*
0417453990000□	0418951057000□	0419156434000*	0420999999000*
0421156434000*	0422951057000□	0423453990000□	0424809017000*
0425707107000*	0426587785000□	0427891007000□	0428309017000*
0429987688000*	0430000000000*	0431987688000□	0432309017000□
0433891007000*	0434587785000*	0435707107000□	0436809017000□
0437453990000*	0438951057000*	0439156434000□	0451000000000□
0452999999000*	0453000000000*	0454999999000□	0455000000000□
0456999999000*	0457000000000*	0458999999000□	0459000000000□
0460999999000*	0461000000000*	0462999999000□	0463000000000□
0464999999000*	0465000000000*	0466999999000□	0467000000000□
0468999999000*	0469000000000*	0470999999000□	0471000000000□
0472999999000*	0473000000000*	0474999999000□	0475000000000□
0476999999000*	0477000000000*	0478999999000□	0479000000000□
0480999999000*	0481000000000*	0482999999000□	0483000000000□
0484999999000*	0485000000000*	0486999999000□	0487000000000□
0488999999000*	0489000000000*	0486999999000□	0487000000000□

TABLE 21. SINE AND COSINE TABLE BY 1/80 INTERVAL (SYMBOLS * AND □ REPRESENT X/0 AND Y/0)

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1089078459000□	1139156434000□	1189233445000□	1239309017000□
1289382683000□	1339453990000□	1389522499000□	1439587785000□
1489649448000□	1539707107000□	1589760406000□	1639809017000□
1689852640000□	1739891007000□	1789923880000□	1839951057000□
1889972370000□	1939987688000□	1989996917000□	1088156434000□
1138309017000□	1188453990000□	1238587785000□	1288707107000□
1338809017000□	1388891007000□	1438951057000□	1488987688000□
1538999999000□	1588987688000□	1638951057000□	1688891007000□
1738809017000□	1788707107000□	1838587785000□	1888453990000□
1938309017000□	1988156434000□	1087233445000□	1137453990000□
1187649448000□	1237809017000□	1287923880000□	1337987688000□
1387996917000□	1437951057000□	1487852640000□	1537707107000□
1587522499000□	1637309017000□	1687078459000□	1737156434000*
1787382683000*	1837587785000*	1887760406000*	1937891007000*
1987972370000*	1086309017000□	1136587785000□	1186809017000□
1236951057000□	1286999999000□	1336951057000□	1386809017000□
1436587785000□	1486309017000□	1536000000000*	1586309017000*
1636587785000*	1686809017000*	1736951057000*	1786999999000*
1836951057000*	1886809017000*	1936587785000*	1986309017000*
1085382683000□	1135707107000□	1185923880000□	1235999999000□
1285923880000□	1335707107000□	1385382683000□	1435000000000*
1485382683000*	1535707107000*	1585923880000*	1635999999000*
1685923880000*	1735707107000*	1785382683000*	1835000000000□
1885382683000□	1935707107000□	1985923880000□	1084453990000□
1134809017000□	1184987688000□	1234951057000□	1284707107000□
1334309017000□	1384156434000*	1434587785000*	1484891007000*
1534999999000*	1584891007000*	1634587785000*	1684156434000*
1734309017000□	1784707107000□	1834951057000□	1884987688000□
1934809017000□	1984453990000□	1083522499000□	1133891007000□
1183996917000□	1233809017000□	1283382683000□	1333156434000*
1383649448000*	1433951057000*	1483972370000*	1533707107000*
1583233445000*	1633309017000□	1683760406000□	1733987688000□
1783923880000□	1833587785000□	1883078459000□	1933453990000*
1983852640000*	1082587785000□	1132951057000□	1182951057000□
1232587785000□	1282000000000*	1332587785000*	1382951057000*
1432951057000*	1482587785000*	1532000000000□	1582587785000□
1632951057000□	1682951057000□	1732587785000□	1782000000000*
1832587785000*	1882951057000*	1932951057000*	1982587785000*
1081649448000□	1131987688000□	1181852640000□	1231309017000□
1281382683000*	1331891007000*	1381972370000*	1431587785000*
1481078459000□	1531707107000□	1581996917000□	1631809017000□
1681233445000□	1731453990000*	1781923880000*	1831951057000*
1881522499000*	1931156434000□	1981760406000□	1080707107000□
1130999999000□	1180707107000□	1230000000000*	1280707107000*

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1330999999000*	1380707107000*	1430000000000□	1480707107000□
1530999999000□	1580707107000□	1630000000000*	1680707107000*
1730999999000*	1780707107000*	1830000000000□	1880707107000□
1930999999000□	1980707107000□	1079760406000□	1129987688000□
1179522499000□	1229309017000*	1279923880000*	1329891007000*
1379233445000*	1429587785000□	1479996917000□	1529707107000□
1579078459000*	1629809017000*	1679972370000*	1729453990000*
1779382683000□	1829951057000□	1879852640000□	1929156434000□
1979649448000*	1078809017000□	1128951057000□	1178309017000□
1228587785000*	1278999999000*	1328587785000*	1378309017000□
1428951057000□	1478809017000□	1528000000000*	1578809017000*
1628951057000*	1678309017000*	1728587785000□	1778999999000□
1828587785000□	1878309017000*	1928951057000*	1978809017000*
1077852640000□	1127891007000□	1177078459000□	1227809017000*
1277923880000*	1327156434000*	1377760406000□	1427951057000□
1477233445000□	1527707107000*	1577972370000*	1627309017000*
1677649448000□	1727987688000□	1777382683000□	1827587785000*
1877996917000*	1927453990000*	1977522499000□	1076891007000□
1126809017000□	1176156434000*	1226951057000*	1276707107000*
1326309017000□	1376987688000□	1426587785000□	1476453990000*
1526999999000*	1576453990000*	1626587785000□	1676987688000□
1726309017000□	1776707107000*	1826951057000*	1876156434000*
1926809017000□	1976891007000□	1075923880000□	1125707107000□
1175382683000*	1225999999000*	1275382683000*	1325707107000□
1375923880000□	1425000000000*	1475923880000*	1525707107000*
1575382683000□	1625999999000□	1675382683000□	1725707107000*
1775923880000*	1825000000000□	1875923880000□	1925707107000□
1975382683000*	1074951057000□	1124587785000□	1174587785000*
1224951057000*	1274000000000□	1324951057000□	1374587785000□
1424587785000*	1474951057000*	1524000000000□	1574951057000□
1624587785000□	1674587785000*	1724951057000*	1774000000000□
1824951057000□	1874587785000□	1924587785000*	1974951057000*
1073972370000□	1123453990000□	1173760406000*	1223809017000*
1273382683000□	1323987688000□	1373078459000□	1423951057000*
1473522499000*	1523707107000□	1573852640000□	1623309017000*
1673996917000*	1723156434000*	1773923880000□	1823587785000□
1873649448000*	1923891007000*	1973233445000□	1072987688000□
1122309017000□	1172891007000*	1222587785000*	1272707107000□
1322809017000□	1372453990000*	1422951057000*	1472156434000□
1522999999000□	1572156434000□	1622951057000*	1672453990000*
1722809017000□	1772707107000□	1822587785000*	1872891007000*
1922309017000□	1972987688000□	1071996917000□	1121156434000□
1171972370000*	1221309017000*	1271923880000□	1321453990000□
1371852640000*	1421587785000*	1471760406000□	1521707107000□
1571649448000*	1621809017000*	1671522499000□	1721891007000□

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1771382683000*	1821951057000*	1871233445000□	1921987688000□
1971078459000*	1070999999000□	1120000000000*	1170999999000*
1220000000000□	1270999999000□	1320000000000*	1370999999000*
1420000000000□	1470999999000□	1520000000000*	1570999999000*
1620000000000□	1670999999000□	1720000000000*	1770999999000*
1820000000000□	1870999999000□	1920000000000*	1970999999000*
1069996917000□	1119156434000*	1169972370000*	1219309017000□
1269923880000□	1319453990000*	1369852640000*	1419587785000□
1469760406000□	1519707107000*	1569649448000*	1619809017000□
1669522499000□	1719891007000*	1769382683000*	1819951057000□
1869233445000□	1919987688000*	1969078459000*	1068987688000□
1118309017000*	1168891007000*	1218587785000□	1268707107000□
1318809017000*	1368453990000*	1418951057000□	1468156434000□
1518999999000*	1568156434000□	1618951057000□	1668453990000*
1718809017000*	1768707107000□	1818587785000□	1868891007000*
1918309017000*	1968987688000□	1067972370000□	1117453990000*
1167760406000*	1217809017000□	1267382683000□	1317987688000*
1367078459000□	1417951057000□	1467522499000*	1517707107000*
1567852640000□	1617309017000□	1667996917000*	1717156434000□
1767923880000□	1817587785000*	1867649448000*	1917891007000□
1967233445000□	1066951057000□	1116587785000*	1166587785000*
1216951057000□	1266000000000*	1316951057000*	1366587785000□
1416587785000□	1466951057000*	1516000000000□	1566951057000□
1616587785000*	1666587785000*	1716951057000□	1766000000000*
1816951057000*	1866587785000□	1916587785000□	1966951057000*
1065923880000□	1115707107000*	1165382683000*	1215999999000□
1265382683000*	1315707107000*	1365923880000□	1415000000000*
1465923880000*	1515707107000□	1565382683000□	1615999999000*
1314309017000*	1364987688000□	1414587785000*	1464453990000*
1114809017000*	1164156434000*	1214951057000□	1264707107000*
1865923880000□	1915707107000*	1965382683000*	1064891007000□
1665382683000□	1715707107000□	1765923880000*	1815000000000□
1514999999000□	1564453990000*	1614587785000*	1664987688000□
1714309017000*	1764707107000*	1814951057000□	1864156434000*
1914809017000*	1964891007000□	1063852640000□	1113891007000*
1163078459000□	1213809017000□	1263923880000*	1313156434000□
1363760406000□	1413951057000*	1463233445000□	1513707107000□
1563972370000*	1613309017000□	1663649448000□	1713987688000*
1763382683000□	1813587785000□	1863996917000*	1913453990000□
1963522499000□	1062809017000□	1112951057000*	1162309017000□
1212587785000□	1262999999000*	1312587785000□	1362309017000□
1412951057000*	1462809017000□	1512000000000*	1562809017000*
1612951057000□	1662309017000*	1712587785000*	1762999999000□
1812587785000*	1862309017000*	1912951057000□	1962809017000*
1061760406000□	1111987688000*	1161522499000□	1211309017000□

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1261923880000*	1311891007000¤	1361233445000*	1411587785000*
1461996917000¤	1511707107000*	1561078459000*	1611809017000¤
1661972370000*	1711453990000¤	1761382683000¤	1811951057000*
1861852640000¤	1911156434000*	1961649448000*	1060707107000¤
1110999999000*	1160707107000¤	1210000000000*	1260707107000*
1310999999000¤	1360707107000*	1410000000000¤	1460707107000¤
1510999999000*	1560707107000¤	1610000000000*	1660707107000*
1710999999000¤	1760707107000*	1810000000000¤	1860707107000¤
1910999999000*	1960707107000¤	1059649448000¤	1109987688000*
1159852640000¤	1209309017000*	1259382683000*	1309891007000¤
1359972370000*	1409587785000¤	1459078459000¤	1509707107000*
1208587785000*	1258000000000¤	1308587785000¤	1358951057000*
1959760406000¤	1058587785000¤	1108951057000*	1158951057000¤
1759923880000*	1809951057000¤	1859522499000*	1909156434000*
1559996917000¤	1609809017000*	1659233445000¤	1709453990000¤
1408951057000¤	1458587785000*	1508000000000¤	1558587785000¤
1608951057000*	1658951057000¤	1708587785000*	1758000000000¤
1808587785000¤	1858951057000*	1908951057000¤	1958587785000*
1057522499000¤	1107891007000*	1157996917000¤	1207809017000*
1257382683000¤	1307156434000¤	1357649448000*	1407951057000¤
1457972370000*	1507707107000¤	1557233445000*	1607309017000*
1657760406000¤	1707987688000*	1757923880000¤	1807587785000*
1857078459000¤	1907453990000¤	1957852640000*	1056453990000¤
1106809017000*	1156987688000¤	1206951057000*	1256707107000¤
1306309017000*	1356156434000*	1406587785000¤	1456891007000*
1506999999000¤	1556891007000*	1606587785000¤	1656156434000*
1706309017000*	1756707107000¤	1806951057000*	1856987688000¤
1906809017000*	1956453990000¤	1055382683000¤	1105707107000*
1155923880000¤	1205999999000*	1255923880000¤	1305707107000*
1355382683000¤	1405000000000*	1455382683000*	1505707107000¤
1555923880000*	1605999999000¤	1655923880000*	1705707107000¤
1755382683000*	1805000000000¤	1855382683000¤	1905707107000*
1955923880000¤	1054309017000¤	1104587785000*	1154809017000¤
1204951057000*	1254999999000¤	1304951057000*	1354809017000¤
1404587785000*	1454309017000¤	1504000000000*	1554309017000*
1604587785000¤	1654809017000*	1704951057000¤	1754999999000*
1804951057000¤	1854809017000*	1904587785000¤	1954309017000*
1053233445000¤	1103453990000*	1153649448000¤	1203809017000*
1253923880000¤	1303987688000*	1353996917000¤	1403951057000*
1453852640000¤	1503707107000*	1553522499000¤	1603309017000*
1653078459000¤	1703156434000¤	1753382683000*	1803587785000¤
1853760406000*	1903891007000¤	1953972370000*	1052156434000¤
1102309017000*	1152453990000¤	1202587785000*	1252707107000¤
1302809017000*	1352891007000¤	1402951057000*	1452987688000¤
1502999999000*	1552987688000¤	1602951057000*	1652891007000¤

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
1702809017000*	1752707107000□	1802587785000*	1852453990000□
1902309017000*	1952156434000□	1051078459000□	1101156434000*
1151233445000□	1201309017000*	1251382683000□	1301453990000*
1351522499000□	1401587785000*	1451649448000□	1501707107000*
1551760406000□	1601809017000*	1651852640000□	1701891007000*
1751923880000□	1801951057000*	1851972370000□	1901987688000*
1951996917000□	1801951057000*	1851972370000□	1901987688000*
0039996917000□	0089987688000□	0139972370000□	0189951057000□
0239923880000□	0289891007000□	0339852640000□	0389809017000□
0439760406000□	0489707107000□	0539649448000□	0589587785000□
0639522499000□	0689453990000□	0739382683000□	0789309017000□
0839233445000□	0889156434000□	0939078459000□	0038987688000□
0088951057000□	0138891007000□	0188809017000□	0238707107000□
0288587785000□	0338453990000□	0388309017000□	0438156434000□
0488000000000*	0538156434000*	0588309017000*	0638453990000*
0688587785000*	0738707107000*	0788809017000*	0838891007000*
0888951057000*	0938987688000*	0037972370000□	0087891007000□
0137760406000□	0187587785000□	0237382683000□	0287156434000□
0337078459000*	0387309017000*	0437522499000*	0487707107000*
0537852640000*	0587951057000*	0637996917000*	0687987688000*
0737923880000*	0787809017000*	0837649448000*	0887453990000*
0937233445000*	0036951057000□	0086809017000□	0136587785000□
0186309017000□	0236000000000*	0286309017000*	0336587785000*
0386809017000*	0436951057000*	0486999999000*	0536951057000*
0586809017000*	0636587785000*	0686309017000*	0736000000000□
0786309017000□	0836587785000□	0886809017000□	0936951057000□
0035923880000□	0085707107000□	0135382683000□	0185000000000*
0235382683000*	0285707107000*	0335923880000*	0385999999000*
0435923880000*	0485707107000*	0535382683000*	0585000000000□
0635382683000□	0685707107000□	0735923880000□	0785999999000□
0835923880000□	0885707107000□	0935382683000□	0034891007000□
0084587785000□	0134156434000□	0184309017000*	0234707107000*
0284951057000*	0334987688000*	0384809017000*	0434453990000*
0484000000000□	0534453990000□	0584809017000□	0634987688000□
0684951057000□	0734707107000□	0784309017000□	0834156434000*
0884587785000*	0934891007000*	0033852640000□	0083453990000□
0133078459000*	0183587785000*	0233923880000*	0283987688000*
0333760406000*	0383309017000*	0433233445000□	0483707107000□
0533972370000□	0583951057000□	0633649448000□	0683156434000□
0733382683000*	0783809017000*	0833996917000*	0883891007000*
0933522499000*	0032809017000□	0082309017000□	0132309017000*
0182809017000*	0232999999000*	0282809017000*	0332309017000*
0382309017000□	0432809017000□	0482999999000□	0532809017000□
0582309017000□	0632309017000*	0682809017000*	0732999999000*
0782809017000*	0832309017000*	0882309017000□	0932809017000□

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0031760406000□	0081156434000□	0131522499000*	0181951057000*
0231923880000*	0281453990000*	0331233445000□	0381809017000□
0431996917000□	0481707107000□	0531078459000□	0581587785000*
0631972370000*	0681891007000*	0731382683000*	0781309017000□
0831852640000□	0881987688000□	0931649448000□	0030707107000□
0080000000000*	0130707107000*	0180999999000*	0230707107000*
0280000000000□	0330707107000□	0380999999000□	0430707107000□
0480000000000*	0530707107000*	0580999999000*	0630707107000*
0680000000000□	0730707107000□	0780999999000□	0830707107000□
0880000000000*	0930707107000*	0029649448000□	0079156434000*
0129852640000*	0179951057000*	0229382683000*	0279453990000□
0329972370000□	0379809017000□	0429078459000□	0479707107000*
0529996917000*	0579587785000*	0629233445000□	0679891007000□
0729923880000□	0779309017000□	0829522499000*	0879987688000*
0929760406000*	0028587785000□	0078309017000*	0128951057000*
0178809017000*	0228000000000□	0278809017000□	0328951057000□
0378309017000□	0428587785000*	0478999999000*	0528587785000*
0578309017000□	0628951057000□	0678809017000□	0728000000000*
0778809017000*	0828951057000*	0878309017000*	0928587785000□
0027522499000□	0077453990000*	0127996917000*	0177587785000*
0227382683000□	0277987688000□	0327649448000□	0377309017000*
0427972370000*	0477707107000*	0527233445000□	0577951057000□
0627760406000□	0677156434000*	0727923880000*	0777809017000*
0827078459000□	0877891007000□	0927852640000□	0026453990000□
0076587785000*	0126987688000*	0176309017000*	0226707107000□
0276951057000□	0326156434000□	0376809017000*	0426891007000*
0476000000000□	0526891007000□	0576809017000□	0626156434000*
0676951057000*	0726707107000*	0776309017000□	0826987688000□
0876587785000□	0926453990000*	0025382683000□	0075707107000*
0125923880000*	0175000000000□	0225923880000□	0275707107000□
0325382683000*	0375999999000*	0425382683000*	0475707107000□
0525923880000□	0575000000000*	0625923880000*	0675707107000*
0725382683000□	0775999999000□	0825382683000□	0875707107000*
0925923880000*	0024309017000□	0074809017000*	0124809017000*
0174309017000□	0224999999000□	0274309017000□	0324809017000*
0374809017000*	0424309017000□	0474999999000□	0524309017000□
0574809017000*	0624809017000*	0674309017000□	0724999999000□
0774309017000□	0824809017000*	0874809017000*	0924309017000□
0023233445000□	0073891007000*	0123649448000*	0173587785000□
0223923880000□	0273156434000*	0323996917000*	0373309017000*
0423852640000□	0473707107000□	0523522499000*	0573951057000*
0623078459000□	0673987688000□	0723382683000□	0773809017000*
0823760406000*	0873453990000□	0923972370000□	0022156434000□
0072951057000*	0122453990000*	0172809017000□	0222707107000□
0272587785000*	0322891007000*	0372309017000□	0422987688000□

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
0472000000000*	0522987688000*	0572309017000*	0622891007000⌑
0672587785000⌑	0722707107000*	0772809017000*	0822453990000⌑
0872951057000⌑	0922156434000*	0021078459000⌑	0071987688000*
0121233445000*	0171951057000⌑	0221382683000⌑	0271891007000*
0321522499000*	0371809017000⌑	0421649448000⌑	0471707107000*
0521760406000*	0571587785000⌑	0621852640000⌑	0671453990000*
0721923880000*	0771309017000⌑	0821972370000⌑	0871156434000*
0921996917000*	0020000000000*	0070999999000*	0120000000000⌑
0170999999000⌑	0220000000000*	0270999999000*	0320000000000⌑
0370999999000⌑	0420000000000*	0470999999000*	0520000000000⌑
0570999999000⌑	0620000000000*	0670999999000*	0720000000000⌑
0770999999000⌑	0820000000000*	0870999999000*	0920000000000⌑
0019078459000*	0069987688000*	0119233445000⌑	0169951057000⌑
0219382683000*	0269891007000*	0319522499000⌑	0369809017000⌑
0419649448000*	0469707107000*	0519760406000⌑	0569587785000⌑
0619852640000*	0669453990000*	0719923880000⌑	0769309017000⌑
0819972370000*	0869156434000*	0919996917000⌑	0018156434000*
0068951057000*	0118453990000⌑	0168809017000⌑	0218707107000*
0468000000000⌑	0518987688000⌑	0568309017000*	0618891007000*
0268587785000*	0318891007000⌑	0368309017000⌑	0418987688000*
0668587785000⌑	0718707107000⌑	0768809017000*	0818453990000*
0868951057000⌑	0918156434000⌑	0017233445000*	0067891007000*
0117649448000⌑	0167587785000⌑	0217923880000*	0267156434000*
0317996917000⌑	0367309017000*	0417852640000*	0467707107000⌑
0517522499000⌑	0567951057000*	0617078459000*	0667987688000⌑
0717382683000*	0767809017000*	0817760406000⌑	0867453990000⌑
0917972370000*	0016309017000*	0066809017000*	0116809017000⌑
0166309017000⌑	0216999999000*	0266309017000⌑	0316809017000⌑
0366809017000*	0416309017000*	0466999999000⌑	0516309017000*
0566809017000*	0616809017000⌑	0666309017000⌑	0716999999000*
0766309017000⌑	0816809017000⌑	0866809017000*	0916309017000*
0015382683000*	0065707107000*	0115923880000⌑	0165000000000*
0215923880000*	0265707107000⌑	0315382683000⌑	0365999999000*
0415382683000⌑	0465707107000⌑	0515923880000*	0565000000000⌑
0615923880000⌑	0665707107000*	0715382683000*	0765999999000⌑
0815382683000*	0865707107000*	0915923880000⌑	0014453990000*
0064587785000*	0114987688000⌑	0164309017000*	0214707107000*
0264951057000⌑	0314156434000*	0364809017000*	0414891007000⌑
0464000000000*	0514891007000*	0564809017000⌑	0614156434000⌑
0664951057000*	0714707107000⌑	0764309017000⌑	0814987688000*
0864587785000⌑	0914453990000⌑	0013522499000*	0063453990000*
0113996917000⌑	0163587785000*	0213382683000*	0263987688000⌑
0313649448000*	0363309017000*	0413972370000⌑	0463707107000*
0513233445000*	0563951057000⌑	0613760406000*	0663156434000*
0713923880000⌑	0763809017000*	0813078459000*	0863891007000⌑

TABLE 21. CONTINUED

ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER	ADDR.	ORDER
0913	852640000*	0012	587785000*	0062	309017000*	0112	951057000□
0162	809017000*	0212	000000000□	0262	809017000□	0312	951057000*
0362	309017000□	0412	587785000□	0462	999999000*	0512	587785000□
0562	309017000□	0612	951057000*	0662	809017000□	0712	000000000*
0762	809017000*	0812	951057000□	0862	309017000*	0912	587785000*
0011	649448000*	0061	156434000*	0111	852640000□	0161	951057000*
0211	382683000□	0261	453990000□	0311	972370000*	0361	809017000□
0411	078459000*	0461	707107000*	0511	996917000□	0561	587785000*
0611	233445000*	0661	891007000□	0711	923880000*	0761	309017000□
0811	522499000□	0861	987688000*	0911	760406000□	0010	707107000*
0060	000000000□	0110	707107000□	0160	999999000*	0210	707107000□
0260	000000000*	0310	707107000*	0360	999999000□	0410	707107000*
0460	000000000□	0510	707107000□	0560	999999000*	0610	707107000□
0660	000000000*	0710	707107000*	0760	999999000□	0810	707107000*
0860	000000000□	0910	707107000□	0009	760406000*	0059	156434000□
0109	522499000□	0159	951057000*	0209	923880000□	0259	453990000*
0309	233445000*	0359	809017000□	0409	996917000*	0459	707107000□
0509	078459000*	0559	587785000*	0609	972370000□	0659	891007000*
0709	382683000□	0759	309017000□	0809	852640000*	0859	987688000□
0909	649448000*	0008	809017000*	0058	309017000□	0108	309017000□
0158	809017000*	0208	999999000□	0258	809017000*	0308	309017000□
0358	309017000□	0408	809017000*	0458	999999000□	0508	809017000*
0558	309017000□	0608	309017000□	0658	809017000*	0708	999999000□
0758	809017000*	0808	309017000□	0858	309017000□	0908	809017000*
0007	852640000*	0057	453990000□	0107	078459000□	0157	587785000*
0207	923880000□	0257	987688000*	0307	760406000□	0357	309017000*
0407	233445000*	0457	707107000□	0507	972370000*	0557	951057000□
0607	649448000*	0657	156434000□	0707	382683000□	0757	809017000*
0807	996917000□	0857	891007000*	0907	522499000□	0006	891007000*
0056	587785000□	0106	156434000*	0156	309017000*	0206	707107000□
0256	951057000*	0306	987688000□	0356	809017000*	0406	453990000□
0456	000000000*	0506	453990000*	0556	809017000□	0606	987688000*
0656	951057000□	0706	707107000*	0756	309017000□	0806	156434000□
0856	587785000*	0906	891007000□	0005	923880000*	0055	707107000□
0105	382683000*	0155	000000000□	0205	382683000□	0255	707107000*
0305	923880000□	0355	999999000*	0405	923880000□	0455	707107000*
0505	382683000□	0555	000000000*	0605	382683000*	0655	707107000□
0705	923880000*	0755	999999000□	0805	923880000*	0855	707107000□
0905	382683000*	0004	951057000*	0054	809017000□	0104	587785000*
0154	309017000□	0204	000000000*	0254	309017000*	0304	587785000□
0354	809017000*	0404	951057000□	0454	999999000*	0504	951057000□
0554	809017000*	0604	587785000□	0654	309017000*	0704	000000000□
0754	309017000□	0804	587785000*	0854	809017000□	0904	951057000*
0003	972370000*	0053	891007000□	0103	760406000*	0153	587785000□
0203	382683000□	0253	156434000□	0303	078459000□	0353	309017000*

TABLE 21. CONTINUED

ADDR. ORDER	ADDR. ORDER	ADDR. ORDER	ADDR. ORDER
040352249000□	045370710700*	050385264000□	055395105700*
060399691700□	065398768800*	070392388000□	075380901700*
080364944800□	085345399000*	090323344500□	000298768800*
005295105700□	010289100700*	015280901700□	020270710700*
025258778500□	030245399000*	035230901700□	040215643400*
045200000000□	050215643400□	055230901700*	060245399000□
065258778500*	070270710700□	075280901700*	080289100700□
085295105700*	090298768800□	000199691700*	005198768800□
010197237000*	015195105700□	020192388000*	025189100700□
030185264000*	035180901700□	040176040600*	045170710700□
050164944800*	055158778500□	060152249900*	065145399000□
070138268300*	075130901700□	080123344500*	085115643400□
090107845900*	075130901700□	080123344500*	085115643400□

IX. APPENDIX C: L.S.II M PROGRAM

A. Form of the L.S.II M Program

1. Modifications made to L.S.II

The modified least squares program (L.S.II M) provides convenient facilities for programming structure factor evaluations involving multiple term structure factors. The Senko and Templeton L.S.II (12) program was designed to handle only single (orthorhombic) term structure factors.

There are four important changes made to the L.S.II program to produce the L.S.II M. A new loading routine is used so that more space is available on the drum for programming. The scale factor storage locations are expanded to allow for a total of 10 scale factors by moving the orders in 0678 and 0679. A small subroutine is inserted just before the make up of arguments section. This subroutine will zero all of the work cells used as temporary storage for the trigonometric term routines. The storage orders for these temporary work cells have been changed to add and store pairs which accumulate results of successive passes through the trigonometric term routines. The orthorhombic terms may be summed in the desired sequence by modifying the term routine exits. This is sufficient for triclinic and monoclinic space groups. For space groups of greater symmetry, a modification of the indices may be made and a new set of terms can be added to the previous results. This may be repeated until the structure factor is obtained. The derivatives of the structure factor are obtained automatically when this procedure is used.

2. Programming information

The trigonometric part of the structure factor should be expressed in the form

$$\sum_{i=1}^{n} \sum_{j=1}^{m} T_{ij}(2\pi\ t_{i1}x)\ T'_{ij}(2\pi\ t'_{i1}y)\ T''_{ij}(2\pi\ t''_{i1}y)$$

where the T_{ij} are either sine or cosine functions, and the t_{i1} are functions of h, k, ℓ. The product of $T_{ij}\ T'_{ij}\ T''_{ij}$ must be one of the available orthorhombic terms. The summation over j is carried out by linking orthorhombic type subroutines and the summation over i is carried out by modifying the t's and repeating the summation over j.

If n = 1, no argument modification is required and a simple modification of the term exits is all that is required. The eight term routines are divided into two types, depending on whether the term is stored as the A or B part of the structure factor. The terms and related information are given in Table 22. For example, if the desired structure factor is $\cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z - \sin 2\pi hx \sin 2\pi ky \sin 2\pi \ell z$, the "A code" on the detail card may be 1408. The exit of the 1408 routine at 1462 is modified to give 21 1704 1558 so that the

Table 22. Orthorhombic structure factor terms

T_{ij}	T'_{ij}	T''_{ij}	Code type	Address	Normal exit	Normal exit order
sine	cosine	cosine	B	1528	1483	21 1729 0796
cosine	sine	cosine	B	1428	1545	21 1729 0796
cosine	cosine	sine	B	1478	1563	21 1729 0796
-sine	sine	sine	B	1578	1971	21 1729 0796
cosine	cosine	cosine	A	1408	1462	21 1704 1999
-cosine	sine	sine	A	1458	1976	21 1704 1999
-sine	cosine	sine	A	1508	1985	21 1704 1999
-sine	sine	cosine	A	1558	1994	21 1704 1999

1558 routine is forced to follow. It should be noted that A code type terms cannot be coupled with B code type terms in this way as different work cells are used.

If a summation over i is required, the procedure is a little more complicated. The summation over j for each i is accomplished in the same manner as above. More than one such pass through the term routines is required in order to sum over i. Each pass must be followed by an argument (t) modification routine which either prepares the new arguments or restores the original conditions and exits to the remainder of the program at 1610. If a new pass through the term routines is required the argument modification routine must exit to 1433 which is the make up of arguments routine. The argument modification routine must be written anew for each new form of the structure factor summation. The first order of the argument modification routine is usually at 1999. The last desired term exit must refer to the start of the appropriate make up of arguments address. The first pass through the term routines is made with the normal indices stored in the following fashion:

0303 has h (t)
0353 has k (t')   with decimal point at 0,
0403 has ℓ (t")

1459 and 1484 have h (t)
1509 and 1534 have k (t')   with decimal point at 2.
1559 and 1584 have ℓ (t")

The argument modification routine operates on these cells to form the new t, t' and t". After the last pass through the term routines these cells and the argument modification routine must be restored to their original condition. There is a short section of the original program which may be used in the argument modification routine. This section will generate the contents of 1459, 1484, 1509, 1534, 1559 and 1584 from the contents of 0303, 0353 and 0403. This routine is entered at 1409 with ℓ (t") in 8003 after locations 0303, 0353 and 0403 have been modified. The normal exit is at 1451 with 24 1459 1894. Since this routine is not needed while the sum over i is carried out, the exit may be modified to 24 1459 XXXX, where XXXX refers to the appropriate argument modification address, when the argument modification routine is first entered. This must be reset before final exit to 1610. Locations 1901 to 1926 and 1937 to 1942 can be used for the modification routine. There are other spaces including part of the atomic band which are available if required. Unless modification is made the program computes the normal orthorhombic structure factor.

The modification cards are loaded with the normal modification cards before the "to S.F." card. The form is

00 000X YYYY word 1 word 2 ... word 7, where X is the number of words to be loaded from the card and YYYY is the address of word 1. The other words are stored sequentially. An exception is 1999, which is loaded with

00 0000 1952 69 1953 1954 word 1 24 1999 1996 .

B. Operating Instructions

1. Assembly of input deck

The deck is loaded in the following sequence:

LS-IIM2 deck,

modification cards,

limit card,
scale factor cards,
standard deviations card,
weighting factor card,
parameter cards,
temperature factor cards,
TO SF card,
CYCLE ZERO cards (5 cards),
a set of detail cards for each layer in the order

KTn card,
reflection cards for nth layer,
NK card.

The last NK card is replaced by an LK card.

2. Console operation

a. Switch settings The console switches are set as follows:

storage entry 70 0001 0003,
programmed not significant,
half cycle run,
address selection not significant,
control run,
display program register,
overflow stop,
error stop.

b. Start program To start the program depress computer reset, program start and start the read feed and the punch feed.

3. Subsequent cycles

With all parameters varying reload input deck beginning with item 10 and start the read feed and the punch feed; do not touch console.

With some parameters held constant or with modification changes place TO LR card in front of the scale factor cards, parameter cards, or temperature cards containing the parameters to be held constant, modification cards and the input deck beginning with item 9. Place this deck in the read feed. Start the read feed and the punch feed but do not touch console.

4. <u>Description of input cards</u>

The NK cards have the form

```
00 0000 0000  61 0832 0692  12 3456 7890  61 0882 0601
00 0000 1394  01 2345 6789  01 2345 6789  00 0000 0000  .
```

The LK card has the form

```
00 0000 0000  61 0832 0692  71 1910 1216  61 0882 0601
69 1107 1956  24 1954 1957  60 0432 1191  00 0000 0000  .
```

The KT"n" card has the form

```
00 0000 0000  60 1633 1953  19 067X 1954  35 0002 1955
21 1632 1394  00 0000 0000  00 0000 0000  00 0000 0000  .
```

The set sums to zero (5 cards) are loaded in the following order:

```
00 0000 0000  24 0332 1953  24 0382 1954  24 0432 1955
24 0482 1956  24 0532 1957  24 0582 1958  24 0632 1394  ,
00 0000 0000  24 0682 1953  24 0932 1954  24 0832 1955
24 1768 1956  24 1793 1957  24 1769 1958  24 1794 1394  ,
00 0000 0000  24 1770 1953  24 1795 1954  24 1771 1955
24 1796 1956  24 1772 0649  69 1958 0642  21 1876 1715  ,
00 0000 0000  69 1951 1953  24 1728 1954  24 1729 1955
24 1726 1956  24 1727 1394  00 0000 0000  00 0000 0000  ,
```

00 0000 0000 69 1953 1954 19 0632 1105 24 1109 1955

69 1956 1957 35 0002 1116 24 1105 1394 00 0000 0000 .

The TO S.F. card has the form

00 0000 1394 ... .

The TO L.R. card has the form

00 0000 0000 00 0000 1996 ... .

The do not punch structure factors card has the form

00 0001 0574 00 0000 1895 ... .

The punch structure factor card has the form

00 0001 0574 71 1927 1895 ... .

The constant weighting factor cards are

00 0001 0354 60 1928 1683 ... ,

00 0001 1378 00 0000 8000 ... .

The above cards do not vary from one calculation to another and may be punched up once and filed with the program deck. The cards described below contain the required information for each structure.

The limit card is 00 0001 1860 20 XXXX 0000 ... , where XXXX = 0250 + 50 n, ($n \leq 16$). n is the number of independent atoms.

The scale factor cards have the form

00 0001 067Y K_y(8) ... , where Y is the layer number ($0 \leq Y \leq 9$).

The standard deviations card is 00 0001 0900 $4\pi^2(u-v)$ (4) ... , where u is the number of independent F values and v is the number of parameters being varied.

The parameter cards have the form

00 0003 bbbb X_n (10) Y_n (10) Z_n (10) ... , where bbbb = 0255 + 50 n, (1 n 16).

The temperature factor cards have the form

00 0002 cccc B_n/λ^2 (5) 19 195X dddd ... , where cccc = 0280 + 50 n, X is the field containing the scattering factors for atom n, dddd is the code controlling the multiplication of the scattering factor by a constant. These factors are listed in Table 23. Other factors may be substituted for these by loading them into the appropriate locations.

Table 23. Multiplicative factors

dddd	Factor	Location
0442	1	-
0317	1/2	0325 (10)
0318	1/4	0326 (10)
0319	1/8	0327 (10)

The reflection cards (detail cards) have the form

hh kk $\ell\ell$ abcd I (7):F (2) $\sin^2\theta$ (10):e f_1 (6):A f_2 (6) f_3 (6) f_4 (6):B f_5 (6) . a, b, and c give the signs of h, k, and ℓ with 8 for plus and 9 for minus. d is 8 for an observed reflection and 9 for unobserved reflections. e is 8 if $F_o \geq 4F_{min}$ and is 9 otherwise. A and B are the structure factor term routine codes as shown in Table 22. The f_i are scattering factors.

5. Description of output cards

Where applicable, all output cards are of the correct format for use as input cards for subsequent cycles if it is necessary to reload the program.

a. Layer output Structure factor cards have the form

$0h0k0\ell \; \begin{matrix}8888\\9999\end{matrix} \; K_yF_o(5) \; : \; \sin^2\theta(4) \; F_c(5) \; F_o\text{-}F_c(5) \; A_o(5)$

$A_o\text{-}A_c(5) \; B_c(5) \; B_o\text{-}B_c(5)$.

Scale factor cards have the form

00 0001 067y $K_y(8)$ $\epsilon K_y(8)$ R_3 for layer (10) .

b. Finish output The reliability factor card is

$R_1(10)$ $R_2(10)$ R_3 all data(10) R_3 last layer (10) .

Atomic cards in sets of three are then punched in the following order:

Temperature factor card

00 0002 cccc $\frac{B_n}{\lambda^2}$ (5) 19 195x dddd $\frac{\epsilon B_n}{\lambda^2}$ (5) ,

Parameter card

00 0003 bbbb $x_n(10)$ $y_n(10)$ $z_n(10)$ $\epsilon x_n(10)$ $\epsilon y_n(10)$ $\epsilon z_n(10)$, and the

Atomic standard deviations card

0 0 0 0 σx_n σy_n σz_n .

R_1, R_2 and R_3 are defined by

$$R_1 = \frac{\Sigma |F_o| - |F_c|}{\Sigma |F_o|}, \quad R_2 = \frac{\Sigma (|F_o| - |F_c|)^2}{\Sigma |F_o|^2}, \text{ and}$$

$$R_3 = \frac{\Sigma w(|F_o| - |F_c|)^2}{\Sigma w|F_o|^2} .$$

6. Plug board

The plug board for the I.B.M. 650 is the same as that used for the L.S.II program which is 8 words straight in and 8 words straight out. A Y-punch in column 1 is used to identify load cards.

7. Program deck

The program cards are listed in Table 24, and must be kept in the order shown. Each line contains the contents of one card.

TABLE 24. PROGRAM CARD LISTING FOR L.S. 2 M (EACH ROW CONTAINS THE CONTENTS OF ONE CARD WITH SYMBOLS * AND ¤ REPRESENTING X/0 AND Y/0)

```
COL.     10        20        30        40        50        60        70        80

000001000¤160001800B690005000D240000000F701851185A650007800B211999000B000000000¤
G01801180A691852185A691854185C691856185E691858185G701895189E691856185H241899189I
F91852180B241895180C691853180D241896180E691854180F241897180G691855180H241898185G
B41996189F701997199G241997189G601951196B241962189H300004197C241973189I441978800A
B41978189F300002199¤241990189G691981196E241981189H240000196A241965189I221981197¤
B41970189F300004198F241986189G151992195¤241992189H691952800B241950189I221987196F
B41966189F601992196H241968189G151981800C241961189H101964196I241964189I000001000¤
B41969189F158001197G241977189G201981198D241984189H111987199A241991189I441995199F
B41995199F108001800C000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007000¤000009990¤009009990¤016009990¤022009990¤028009990¤034009990¤041009990¤
000007000G047009990¤053009980¤060009980¤066009980¤072009970¤078009970¤085009960¤
000007001D091009960¤097009950¤103009940¤110009940¤116009930¤122009920¤128009910¤
000007002A135009910¤141009900¤147009890¤153009880¤159009870¤166009860¤172009850¤
000007002H178009840¤184009820¤190009810¤197009800¤203009790¤209009780¤215009760¤
000007003E221009750¤227009740¤233009720¤240009710¤246009690¤252009680¤258009660¤
000007004B264009640¤270009630¤276009610¤282009590¤288009580¤294009560¤300009540¤
000007004I306009520¤312009500¤318009480¤324009460¤330009440¤336009420¤342009400¤
000007005F348009380¤353009350¤359009330¤365009310¤371009280¤377009260¤383009240¤
000007006C388009210¤394009190¤400009160¤406009140¤411009110¤417009090¤423009060¤
000007007¤429009030¤434009000¤440008980¤445008950¤451008920¤457008890¤462008860¤
000007007G468008830¤473008800¤479008770¤484008740¤490008710¤495008680¤501008650¤
000007008D506008620¤511008590¤517008560¤522008520¤528008490¤533008460¤538008420¤
000007009A543008390¤549008360¤554008320¤559008290¤564008250¤569008220¤575008180¤
000007009H580008140¤585008110¤590008070¤595008030¤600008000¤605007960¤610007920¤
000007010E615007880¤620007840¤625007800¤630007770¤635007730¤639007690¤644007640¤
000007011B649007600¤654007560¤659007520¤663007480¤668007440¤673007400¤677007350¤
000007011I682007310¤687007270¤691007220¤696007180¤700007140¤705007090¤709007050¤
000007012F714007000¤718006960¤722006910¤727006870¤731006820¤735006770¤740006730¤
000007013C744006680¤748006630¤752006590¤756006540¤760006490¤764006440¤769006390¤
000007014¤773006350¤777006300¤780006250¤784006200¤788006150¤792006100¤796006050¤
000007014G800006000¤803005950¤807005900¤811005850¤814005800¤818005750¤822005690¤
```

TABLE 24. CONTINUED

```
COL.    10        20        30        40        50        60        70        80

000007015D825005640¤829005590¤832005540¤836005490¤839005430¤842005380¤846005330¤
000007016A849005280¤852005220¤856005170¤859005110¤862005060¤865005010¤868004950¤
000007016H871004900¤874004840¤877004790¤880004730¤883004680¤886004620¤889004570¤
000007017E892004510¤895004450¤898004400¤900004340¤903004290¤906004230¤909004170¤
000007018B911004110¤914004060¤916004000¤919003940¤921003880¤924003830¤926003770¤
000007018I928003710¤931003650¤933003590¤935003530¤938003480¤940003420¤942003360¤
000007019F944003300¤946003240¤948003180¤950003120¤952003060¤954003000¤956002940¤
000007020C958002880¤959002820¤961002760¤963002700¤964002640¤966002580¤968002520¤
000007021¤969002460¤971002400¤972002330¤974002270¤975002210¤976002150¤978002090¤
000007021G979002030¤980001970¤981001900¤982001840¤984001780¤985001720¤986001660¤
000007022D987001590¤988001530¤989001470¤990001410¤991001350¤991001280¤992001220¤
000007023A993001160¤994001100¤994001030¤995000970¤996000910¤996000850¤997000780¤
000007023H997000720¤998000660¤998000600¤998000530¤999000470¤999000410¤999000340¤
000007024E999000280¤999000220¤999000160¤999000090¤999000030¤999000000¤951610000¤
000007025B861109048D779108187C705007408B637906703B577206065C522305488A472504965H
000007025I427604493C386904065G350103678H316803328G286603011I259302725C234702466¤
000007026F212302231C192202019¤173801826H157301653¤142301495G128801353D116601224F
000007027C105401108¤095401002F086400907B078100820H070600742G064000672A057900608A
000007028¤052300550B047400497I042900450E038800407F035100368H031700333G028800302¤
000007028G026000273B023500247B021300223G019200202D017500183B015700165G014300150¤
000007029D012900135G011700122H010600111A009500100E008700091¤007800082C007100074E
000004030A006400067D100332035B000000000C601559156F008700091¤007800082C007100074E
000007031G608003032B608003032C608003032D201927163A000000195B190325044B190326044B
000006032D190327044B500000000¤250000000¤125000000¤668002163H191582141C190326044B
000007034A191654142A210303135G072000000*241550144E241550152¤241550140C241550145C
000007034H210353136¤600523042G600403150G658002176¤210332035D000000000K691953081H
000007036G608003037B608003037C608003037D350002147G608003178G190425044B190426044B
000006037D190427044B062500000¤031250000¤015625000¤668002163G191582148H190426044B
000007039A191604147A210517052¤460396039G211770175B211603160G691699185C691650185C
000007039H211771039I601603164H000017676D108001042E691927074H000000000D600517047E
000007041G101770039D101771039H101772179H191380154F101726039B191767161G241576142¤
000006042D211928030B210382034I191632042D198001138C690382044D191532141C241576142¤
```

TABLE 24. CONTINUED

```
COL.     10        20        30        40        50        60        70        80

000007044A191654152A210447140¤000000000¤350002040A040000000¤210400040D000091588¤
000007044H241851171¤678003061I200432049I108001047F000012256E350004037A101928040B
000007046G690420042C191379144F191380149F191379159F241576142¤241576149E241576149E
000006047D690477139B198001138A210482049H300002057B690482049C191532148H241576149E
000007049A191604157A100445800C350002045A618002045D000099246E200452061G150400047D
000007049H600523169D601930138E191930138G210632059E110517052I601612057¤211612051I
000007051G000000000¤698003052D198001057I600523139C123456789¤191928071G000000000¤
000006052D231378138D191378057E198001057G211932054H211933050B211934055B000000000¤
000007054A600495135B190495059I601378054D191928059G608002050D210532050C110523052G
000007054H600452052B210582054C240523055A211772171E601378050¤240517062¤608002056I
000007056G350005042F691928138F210573052F190573057H100682059C160625067I000698280¤
000006057D711927189E201680054A241936057D100532054F100632050A100582054I000698280¤
000007059A690551059B241798171E210682059A690443055C651953056H231928073B300002055D
000007059H641929049F201755179G000001067A100582060B240882060C640782069F000001000¤
000007061G608002052E190573057A150432045¤240523057F651957071I690825067H601928074A
000006062D000000000¤000001000¤000000000¤000000000¤230795800A690641064D601928074A
000007064A211772162E241861064E600749090D241798139D690646064G461868064H241865171E
000007064H690650065A240882195G211876187I241861065B690653070A461868182¤350004086G
000007066G350004137G690718072A100000000¤036479845H012575551I023741905C007394878¤
000006067D006718064B000000000¤000000000¤000000000¤241378069I460891074B007394878¤
000007069A240694195C100532069C240832069E000000000¤210782074C201930069G711910195E
000007069H711910120C601928168C190340084C241865182¤690718077A310004077E210870087C
000007071G350004052H000001163C698003062H210000000¤230600077D201928070B610682079C
000006072D211928074E210770082C000000000¤210749119¤190746077B151633082B610682079C
000002073B201888059D000000000¤000000000¤210749119¤190746077B151633082B610682079C
000007074A110794084I158001085¤660932079B608002075C650749085D700000000*350002080D
000007074H910802085C210670072D350004076G300004076H200447140¤191632075A240932075¤
000007076G640782074D608002072H608002077I000000005C241927089B211929079I241927118¤
000006077D241927064C608002128F000000000¤000000000¤690443079G191633070C241927118¤
000007079A190340074G150632075D198001080C000010000¤000000000¤651954071I241851087A
000007079H310008091G101632074I000000000¤000000000¤211930044I350002081G210720072C
000007081G100720072E910622062C201930049H777777777G201378069I201633072B440829084A
```

TABLE 24. CONTINUED

```
COL.     10        20        30        40        50        60        70        80

000006082D641928082A000000040¤000000000¤000000000¤000000000¤600632070¤440829084A
000007084A690820077C190312065D350004070D000000000¤000000000¤000000000¤000000000¤
000007084H000000000¤460622085B201929049D000000000¤650669082D460868081I300004066H
000007086G100870079H611929080B000000000¤000000000¤241876173C000000000¤610682084B
000006087D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤610682084B
000007089A241929049D711910110¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007089H000000000¤000000000¤400000000¤000000000¤000000000¤000000000¤100604072G
000007091G640770076I000000000¤000000000¤000000600¤000000000¤000000000¤000000000¤
000006092D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007094A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007094H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007096G000000000¤000000000¤000000000¤000000900¤000000000¤000000000¤000000000¤
000006097D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000001098B000000200¤690305180H690308181A111852800C211936194¤601897800C601898800C
000007099A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007099H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007101G000000000¤000000000¤000000000¤000000020¤000000000¤000000000¤000000000¤
000006102D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007104A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007104H000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007106G000000000¤000000000¤000000000¤000010000¤000000000¤000000000¤000000000¤
000006107D000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007109A000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000007109H000000000¤000000000¤600532113G101158114F101158114H000000000¤350002111G
000007110E350001111F241934114¤711910120C241928113D190312110E000000000¤241929118B
000007111B190920111C210870120E210870118C100870116E100870112E210870112C691171112F
000007111I310004113¤000017000¤310001112I241020112G610682110I201929120A310001113F
000007112F231171117D198001116G201931120H640982112D691283128G241070113C191070114G
000007113C191020115B600920113B000000000¤640770112I190312110D000000000¤210870120G
000007114¤711910132I000000000¤441146110A711910195D441148110B640382117B210920120D
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```

148

TABLE 24. CONTINUED

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COL.     10        20        30        40        50        60        70        80

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000007136D668002032¤690468047A690469047B690470047C241575035¤198001135F461382139¤
000007137A648001136B961637037H951638032H000000000¤300004059H641929164¤211931054G
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TABLE 24. CONTINUED

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000007140F611559141F191761143E601561136E608003037¤350002147E000000000¤000000000¤
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000007142G000000000¤601582143G611484159A611534148I611584144A000000000¤000000000¤
000007143D691663152E691538169B000000000¤690341034D608002144E691442167A691443162A
000007144A691444162B191380147C191379152B191380152D191500159E211701140D211702140E
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TABLE 24. CONTINUED

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TABLE 24. CONTINUED

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COL.     10        20        30        40        50        60        70        80

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TABLE 24. CONTINUED

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COL.     10         20         30         40         50         60         70         80

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000004157A101726158F101727196C101728196G101729197A000000000¤000000000¤000000000¤
000001158F211726157I000000000¤000000000¤000000000¤000000000¤000000000¤000000000¤
000004159F101701198H101702198I101703199C101704199D000000000¤000000000¤000000000¤
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000000195B691953195D000000161¤241999199F000000000¤000000000¤000000000¤000000000¤
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```

X. APPENDIX D: STRUCTURE FACTORS

The observed and calculated structure factor amplitudes for the erbium, yttrium and praseodymium ethylsulfates are given in Tables 25, 26 and 27 respectively of this appendix. An L is inserted in the value of F_o for unobserved reflections to indicate that the value given is that for F_{min}. If F_o is left blank, the reflection intensity was not measured.

TABLE 25. STRUCTURE FACTORS FOR ERBIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES ≤ AND K = 1.2)

H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C
H	1	0	6	151	152	13	L49	9-	4	58	54-	H	11	0
0		226-	7	100	89-	14	68	58	5	130	142	0	121	107-
1		192	8	107	104-	15	L53	20-	6	45	45-	1	80	74-
2		20-	9	110	112	16	L55	21-	7	42	37-	2	96	104
3	131	125-	10	55	62-	H	6	0	8	130	121	3	93	98-
4	206	207	11	58	64-	0	327	304	9	56	47-	4	43	49-
5	77	79-	12	85	100	1	311	293-	10	L48	21-	5	87	105
6	135	133-	13	L46	30-	2	L29	8	11	66	74	6	52	41-
7	368	358	14	63	78-	3	183	178	12	L52	12-	7	48	28-
8	46	38-	15	84	110	4	85	84-	13	L54	23-	8	75	77
9	137	131-	16	L52	23-	5	129	126-	14	L56	53	9	L52	14-
10	148	171	17	L55	44-	6	60	79	15	L58	22-	10	L53	18-
11	78	77-	18	69	68	7	63	58-	16	L59	28-	11	L56	54
12	58	56-	H	4	0	8	90	93-	H	9	0	12	L56	15-
13	81	99	0	187	172-	9	116	127	0	206	191	H	12	0
14	64	67-	1	256	237	10	54	63-	1	69	77-	0	123	131
15	63	63-	2	220	204-	11	77	81-	2	51	42-	1	68	61-
16	75	94	3	68	69-	12	94	106	3	110	104	2	59	61-
17	52	49-	4	180	183	13	L51	35-	4	67	67-	3	69	77
H	2	0	5	61	47	14	L53	41-	5	70	71-	4	75	68-
0		176-	6	187	190-	15	82	91	6	85	100	5	78	73-
1		288-	7	140	147	16	L56	25-	7	73	77-	6	59	69
2	80	82	8	L36	22-	H	7	0	8	69	70-	7	50	45-
3	208	195-	9	64	56-	0	182	169-	9	87	106	8	52	41-
4	95	80-	10	116	128	1	212	238	10	66	64-	9	66	66
5	227	250	11	64	69-	2	95	91-	11	57	49-	10	68	52-
6	173	166-	12	64	66-	3	175	176-	12	66	81	11	L57	20-
7	161	160-	13	67	81	4	222	242	13	L56	34-	12	72	52
8	215	237	14	65	57-	5	L36	27-	14	L58	26-	H	13	0
9	156	152-	15	52	53-	6	152	147-	15	L58	65	0	42	35-
10	38	37-	16	L53	51	7	148	156	16	73	26-	1	126	133
11	125	147	H	5	0	8	87	78-	H	10	0	2	45	50-
12	94	94-	0	43	31	9	93	94-	0	119	109-	3	L46	19-
13	L33	1-	1	194	197-	10	124	129	1	204	210	4	130	128
14	96	108	2	172	176	11	63	58-	2	89	79-	5	49	43-
15	65	66-	3	89	90-	12	71	65-	3	L39	11	6	51	36-
16	L52	29-	4	110	101-	13	52	56	4	157	171	7	69	90
17	53	66	5	192	199	14	L55	39-	5	67	69-	8	L53	40-
H	3	0	6	113	112-	15	L57	41-	6	62	73-	H	14	0
0	391	446	7	L36	12-	16	L57	52	7	137	146	0	80	76-
1	280	267-	8	167	177	H	8	0	8	L48	56-	1	79	76-
2	190	153	9	73	90-	0	79	66-	9	L50	51-	2	90	94
3	232	256	10	L43	8	1	211	211-	10	73	80	3	48	35-
4	226	218-	11	95	103	2	192	200	11	L54	46-	4	50	52-
5	28	11	12	47	28-	3	107	99-	12	L55	30-	5	L51	62

TABLE 25. CONTINUED

H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C
6	L53	6-	9	164	153	11	76	70	H	6	1	11	L42	16
7	L54	40-	10	L30	10	12	L37	11	0	L22	17-	12	53	63-
8	62	68	11	152	153-	13	118	97-	1	250	264-	13	56	61
H	15	0	12	156	156	14	L40	43	2	154	153	14	L47	15
0	99	101	13	L36	16	15	L43	6-	3	29	26	H	9	1
1	48	47-	14	116	113-	16	77	67-	4	120	119-	0	37	32
2	69	56-	15	122	114	17	52	52	5	111	113	1	151	145-
3	66	75	16	L42	2-	18	48	2	6	L30	16	2	141	152
4	52	40-	17	94	91-	H	4	1	7	100	96-	3	54	50
5	65	53-	18	69	65	0	135	149	8	72	66	4	104	111-
6	54	52	19	48	10-	1	23	35-	9	L35	6	5	99	91
7	L56	39-	20	69	52-	2	53	60-	10	123	118-	6	44	38
H	16	0	21	50	40	3	109	128	11	48	66	7	122	120-
0	49	19-	H	2	1	4	99	94-	12	41	2	8	62	62
1	106	108	0		325-	5	150	161-	13	91	84-	9	L40	15
2	62	47-	1	210	273	6	179	196	14	44	44	10	82	84-
3	52	19-	2	176	174	7	105	81	15	L35	1	11	48	46
4	53	71	3	238	276-	8	142	134-	16	48	54-	12	72	3
5	L55	26-	4	263	309	9	173	167	H	7	1	13	53	67-
6	L57	22-	5	L22	24-	10	L35	14	0	85	79	14	54	48
7	57	52	6	258	282-	11	111	110-	1	61	34	H	10	1
H	17	0	7	128	137	12	125	126	2	175	179-	0	126	122
0	51	46-	8	35	27-	13	L40	12-	3	121	122	1	30	21-
1	52	53-	9	216	221-	14	73	72-	4	L29	20	2	140	141-
2	53	69	10	149	142	15	85	84	5	166	161-	3	127	119
3	L54	28-	11	L34	6	16	L45	16-	6	163	166	4	L35	4
4	L56	38-	12	104	98-	17	53	57-	7	L34	16	5	107	97-
5	64	63	13	94	84	18	48	48	8	94	101-	6	104	101
H	18	0	14	L39	3	H	5	1	9	139	139	7	L39	8-
0	92	88	15	66	68-	0	294	332-	10	L39	6-	8	67	55-
1	54	37-	16	81	67	1	282	316	11	58	60-	9	92	89
2	55	31-	17	L45	15	2	32	33-	12	100	91	10	L44	5-
3	56	58	18	47	41-	3	220	249-	13	L44	19-	11	L45	42-
H	19	0	19	48	40	4	234	248	14	L46	55-	12	53	54
0	55	17-	H	3	1	5	30	24-	H	8	1	13	48	14-
1	56	51	0	140	151	6	211	219-	0	195	196-	H	11	1
H	1	1	1	144	159-	7	160	156	1	195	195	0	134	125-
0		263	2	209	231	8	54	40-	2	49	38-	1	124	114
1		292-	3	L21	24	9	104	104-	3	148	141-	2	63	52-
2		319-	4	128	128-	10	102	96	4	145	161	3	112	107-
3	128	142	5	155	165	11	L38	4-	5	58	54-	4	95	90
4	L19	3-	6	71	54	12	85	74-	6	121	126-	5	38	35-
5	287	318-	7	62	57-	13	85	78	7	103	103	6	88	82-
6	139	149	8	104	104	14	44	16	8	37	17-	7	79	79
7	31	18	9	71	42-	15	50	52-	9	98	105-	8	47	24-
8	187	177-	10	102	92-	16	52	54	10	86	90	9	72	72-

TABLE 25. CONTINUED

H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C	H	KF_O	KF_C
10	L45	60	1	L42	7-	13	100	102-	H	4	2	7	121	121
11	L47	6	2	53	51-	14	43	47	0	137	141	8	85	75
H	12	1	3	67	64	15	71	63	1	350	373-	9	104	105-
0	L34	28	4	30	1-	16	53	73-	2	L23	18	10	66	65
1	100	92-	5	52	47-	17	60	43	3	146	155	11	73	64
2	138	133	H	17	1	18	L51	28	4	242	271-	12	102	97-
3	L37	31	0	65	64-	H	2	2	5	L28	14-	13	47	57
4	110	104-	1	54	47	0		209	6	100	98	14	L49	29
5	116	104	2	12	1-	1	253	292	7	191	183-	15	93	85-
6	41	27	3	57	61-	2	196	227-	8	L35	18	H	7	2
7	88	86-	4	53	44	3	123	129	9	82	78	0	129	121
8	66	65	5	48	3-	4	170	175	10	152	153-	1	162	148-
9	45	3	H	18	1	5	203	219-	11	L40	34	2	45	40
10	78	75-	0	L32	1	6	111	105	12	90	81	3	132	126
11	53	49	1	61	58-	7	65	60	13	98	95-	4	246	295-
H	13	1	2	78	70	8	148	156-	14	77	66	5	96	86
0	90	77	3	48	3-	9	85	88	15	L48	43	6	98	98
1	36	8	4	L49	48-	10	74	68	16	57	59-	7	156	152-
2	113	102-	5	55	49	11	175	170-	17	L52	27	8	66	56
3	112	107	H	19	1	12	53	53	H	5	2	9	66	64
4	40	10	0	L47	46	13	L42	21	0	162	174	10	108	110-
5	69	68-	1	L48	1	14	106	104-	1	202	218	11	56	56
6	74	72	2	54	47-	15	46	52	2	130	120-	12	47	48
7	L44	7	H	20	1	16	48	17	3	146	145	13	55	66-
8	L45	39-	0	54	52-	17	56	62-	4	50	44	H	8	2
9	62	56	1	L49	36	18	L52	36	5	177	170-	0	96	76
10	54	3	2	49	2	H	3	2	6	200	189	1	106	109
H	14	1	H	21	1	0	226	263-	7	L34	4-	2	87	72-
0	82	84-	0	L50	2-	1	67	73	8	172	160-	3	130	120
1	61	58	1	50	30-	2	253	271	9	57	57	4	46	55
2	56	26-	H	0	2	3	293	324-	10	L40	32	5	106	106-
3	71	74-	0		582-	4	123	126	11	125	107-	6	42	34
4	L42	51	H	1	2	5	149	142	12	L44	33	7	39	41
5	48	13-	0		4	6	160	170-	13	L46	8	8	58	65-
6	74	67-	1		137-	7	166	164	14	77	72-	9	L43	26
7	46	47	2	66	44-	8	130	121	15	L50	36	10	L45	28
8	53	3-	3	148	176	9	142	136-	16	L52	20	11	67	73-
H	15	1	4	288	312-	10	88	78	17	54	50-	12	L49	25
0	L39	20	5	L24	26	11	124	108	H	6	2	13	L51	27
1	105	88-	6	50	46	12	106	101-	0	212	239-	H	9	2
2	114	100	7	169	179-	13	43	39	1	155	143	0	100	106-
3	L43	10	8	63	39-	14	60	65	2	36	36	1	36	11
4	93	81-	9	77	82	15	86	86-	3	195	207-	2	37	38
5	L45	66	10	124	122-	16	L49	25	4	176	172	3	150	146-
H	16	1	11	L36	36	17	51	47	5	89	88	4	48	54
0	80	73	12	103	97	18	59	65-	6	139	141-	5	86	70

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
6	94	89-	9	84	72-	6	L53	16	0		246	8	98	90
7	46	57	10	52	41	7	L54	39-	1	113	132-	9	151	149-
8	43	39	11	L54	28	8	56	27	2	58	57-	10	L34	17-
9	78	79-	H	13	2	H	17	2	3	217	246	11	98	86
10	62	53	0	74	68	0	L48	29	4	127	144-	12	110	107-
11	59	47	1	157	147-	1	L49	41	5	L22	6	13	L19	1
12	88	81-	2	46	57	2	67	66-	6	244	266	14	78	64
13	52	28	3	48	34	3	L51	24	7	57	65-	15	83	78-
H	10	2	4	146	131-	4	58	38	8	L28	5	16	L45	8
0	140	126	5	92	74	5	66	64-	9	217	233	17	57	55
1	212	206-	6	L47	20	6	L55	19	10	119	122-	H	5	3
2	72	64	7	92	86-	7	L56	19	11	L34	11-	0	242	277
3	69	55	8	57	44	8	63	47-	12	122	116	1	191	218-
4	201	195-	9	L52	34	H	18	2	13	83	86-	2	42	30
5	64	66	10	L54	51-	0	67	66-	14	43	6	3	224	236
6	63	57	11	L55	28	1	L51	27	15	65	64	4	180	182-
7	125	116-	H	14	2	2	L52	43	16	67	64-	5	42	33
8	56	49	0	66	59	3	65	61-	17	44	7-	6	212	221
9	46	41	1	67	73	H	19	2	H	3	3	7	134	131-
10	69	75-	2	83	84-	0	L52	14	0	84	101-	8	50	38
11	L50	35	3	51	30	1	53	51-	1	70	78	9	128	121
12	L52	37	4	L46	44	H	20	2	2	167	203-	10	94	88-
H	11	2	5	59	73-	0	54	30	3	91	76-	11	L37	11
0	119	103	6	L49	23	H	1	3	4	86	92	12	81	79
1	100	92	7	57	37	0		193-	5	160	149-	13	84	76-
2	100	98-	8	78	70-	1		42	6	78	62-	14	42	3-
3	58	55	9	L54	12	2	231	316	7	43	48	15	50	49
4	102	90	10	L55	31	3	211	246-	8	98	100-	H	6	3
5	95	91-	11	62	48-	4	46	42-	9	L31	24	0	L22	17-
6	44	32	H	15	2	5	231	269	10	104	91	1	113	134
7	L46	32	0	69	70-	6	187	215-	11	74	67-	2	119	117-
8	70	72-	1	L45	25	7	L25	3-	12	L36	13-	3	92	77-
9	L48	12	2	52	48	8	98	105	13	112	91	4	93	87
10	50	39	3	67	73-	9	159	160-	14	L40	40-	5	127	120-
11	74	62-	4	73	49	10	L30	9-	15	L42	6	6	54	43-
12	54	15	5	56	46	11	110	110	16	69	63	7	98	90
H	12	2	6	63	58-	12	144	142-	17	L45	47-	8	84	78-
0	154	146-	7	L53	39	13	L36	25-	H	4	3	9	L35	17-
1	L38	29	8	L54	23	14	87	91	0	145	170-	10	118	105
2	109	91	H	16	2	15	103	99-	1	L18	6-	11	82	72-
3	119	99-	0	L46	10	16	L42	6-	2	168	170	12	L25	1-
4	57	51	1	82	85-	17	92	79	3	185	193-	13	79	74
5	73	63	2	68	55	18	55	60-	4	100	107	14	49	48-
6	79	77-	3	L49	11	19	L47	5	5	140	138	15	L32	1
7	53	49	4	72	69-	20	54	49	6	205	214-	H	7	3
8	L49	37	5	52	36	H	2	3	7	41	28-	0	81	81-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
1	L25	19	14	67	45-	5	58	63	H	19	3	13	L43	4-
2	191	185	H	10	3	6	82	64-	0	51	47-	14	106	96
3	139	130-	0	104	105-	7	L43	4-	1	L47	4-	15	57	51-
4	54	41	1	48	43	8	L45	39	2	L47	46	H	3	4
5	149	133	2	133	139	9	L46	50-	3	54	44-	0	163	222
6	152	143-	3	112	101-	10	L47	4-	H	20	3	1	111	125-
7	L34	8	4	L34	13	H	14	3	0	47	47	2	37	28-
8	81	75	5	93	87	0	64	63	1	L48	30-	3	160	188
9	99	106-	6	90	76-	1	60	60-	H	21	3	4	140	149-
10	L38	4	7	38	13	2	39	24	0	48	1	5	76	80-
11	49	53	8	49	49	3	40	55	1	L49	29	6	133	147
12	78	78-	9	66	69-	4	41	48-	H	0	4	7	117	111-
13	L43	12	10	L43	2	5	47	9	0		617	8	107	103-
14	L45	54	11	44	46	6	69	56	H	1	4	9	107	104
15	57	54-	H	11	3	7	45	44-	0		125-	10	95	82-
H	8	3	0	103	99	8	46	2-	1		219	11	63	52-
0	143	153	1	122	127-	9	L47	45	2		42-	12	69	77
1	178	178-	2	38	41	10	68	45-	3	37	46-	13	L44	38-
2	28	35	3	103	87	H	15	3	4	160	179	14	65	59-
3	136	125	4	103	88-	0	L38	20-	5	53	54-	15	83	82
4	158	151-	5	42	26	1	98	91	6	63	57-	H	4	4
5	64	49	6	70	65	2	100	89-	7	210	229	0	89	92-
6	106	115	7	70	72-	3	L42	5-	8	31	15-	1	175	214
7	90	90-	8	L42	17	4	91	81	9	97	91-	2	79	83-
8	L37	17	9	74	64	5	70	65-	10	135	123	3	40	43-
9	94	95	10	50	56-	6	L45	5	11	46	46-	4	167	178
10	90	81-	11	L46	9-	7	57	55	12	56	59-	5	53	42
11	L42	10-	H	12	3	H	16	3	13	90	84	6	117	118-
12	57	60	0	60	40-	0	70	68-	14	53	51-	7	147	137
13	50	56-	1	113	104	1	L42	2	15	60	60-	8	L36	7-
14	L46	10-	2	119	114-	2	L42	47	16	79	82	9	59	45-
H	9	3	3	45	41-	3	72	63-	17	56	44-	10	115	114
0	72	57-	4	123	112	4	L27	1	H	2	4	11	46	47-
1	112	107	5	110	104-	5	46	43	0		174-	12	48	56-
2	106	116-	6	L40	20-	H	17	3	1	123	159-	13	78	76
3	98	84-	7	102	83	0	L42	49	2	111	128	14	L47	46-
4	114	116	8	75	67-	1	48	39-	3	156	173-	15	69	44-
5	103	94-	9	L43	1	2	L10	1	4	39	37-	H	5	4
6	50	50-	10	73	68	3	50	52	5	157	175	0	100	107-
7	129	112	11	58	47-	4	L46	38-	6	128	119-	1	109	119-
8	77	70-	H	13	3	H	18	3	7	92	88-	2	113	107
9	L40	13-	0	81	73-	0	L05	1	8	153	175	3	120	118-
10	66	75	1	L36	6-	1	55	57	9	99	98-	4	81	60-
11	48	51-	2	118	96	2	65	64-	10	36	28-	5	108	114
12	L44	2-	3	118	94-	3	L46	4	11	137	126	6	87	85-
13	65	57	4	L39	4-	4	47	47	12	65	65-	7	L35	21-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
8	134	125	8	104	92	0	112	111	5	76	56	H	3	5
9	67	61-	9	L44	37-	1	L39	40-	H	18	4	0	38	49
10	L41	10-	10	L46	31-	2	46	45-	0	80	69	1	96	112-
11	96	89	11	53	66	3	69	73	1	57	29-	2	122	154
12	L45	24-	12	L49	16-	4	53	49-	H	19	4	3	L27	2-
13	L46	15-	H	9	4	5	71	56-	0	L52	14-	4	70	80-
14	59	56	0	148	165	6	56	65	1	53	45	5	121	120
H	6	4	1	52	47-	7	47	35-	H	20	4	6	L34	29
0	194	222	2	L35	31-	8	49	33-	0	60	27-	7	61	56-
1	148	158-	3	111	107	H	13	4	H	1	5	8	87	79
2	L28	33-	4	59	53-	0	49	48-	0		175	9	L41	26-
3	161	165	5	55	52-	1	121	119	1		128-	10	69	68-
4	90	80-	6	96	93	2	60	59-	2	119	175-	11	51	56
5	107	106-	7	66	64-	3	L44	20-	3	90	106	12	L48	3
6	94	92	8	62	50-	4	114	105	4	25	23-	13	80	73-
7	66	72-	9	103	88	5	L46	47-	5	176	183-	14	53	38
8	75	71-	10	58	52-	6	54	27-	6	115	116	15	L55	3-
9	104	104	11	L49	38-	7	L49	70	7	L33	12	H	4	5
10	60	64-	12	72	67	8	L51	35-	8	129	136-	0	75	96
11	70	59-	H	10	4	H	14	4	9	124	121	1	43	37-
12	74	81	0	121	116-	0	47	55-	10	L40	9	2	71	67-
13	48	32-	1	172	185	1	53	59-	11	114	111-	3	90	93
H	7	4	2	98	73-	2	81	78	12	109	114	4	L31	45-
0	147	139-	3	L37	11-	3	L46	25-	13	L48	9	5	122	118-
1	201	206	4	144	151	4	L48	46-	14	94	87-	6	116	130
2	47	49-	5	76	68-	5	L48	57	15	91	87	7	54	50
3	138	132-	6	52	54-	6	L50	5-	16	L55	2-	8	105	100-
4	199	216	7	131	119	7	L51	36-	17	80	71-	9	127	123
5	39	26-	8	56	50-	8	75	61	H	2	5	10	46	5
6	109	102-	9	L48	38-	H	15	4	0		205-	11	86	81-
7	137	141	10	60	66	0	80	79	1	132	180	12	96	95
8	76	60-	11	51	36-	1	65	33-	2	64	70	13	L52	8-
9	76	68-	H	11	4	2	74	48-	3	153	177-	14	66	58-
10	113	110	0	97	90-	3	58	65	4	170	190	15	63	64
11	56	45-	1	46	55-	4	L49	30-	5	L30	13-	H	5	5
12	58	50-	2	66	70	5	L50	46-	6	193	195-	0	177	199-
13	49	53	3	75	69-	H	16	4	7	117	113	1	183	207
H	8	4	4	L41	50-	0	L46	20-	8	L37	17-	2	L30	21-
0	114	108-	5	77	80	1	107	91	9	145	153-	3	171	170-
1	120	132-	6	45	30-	2	L48	48-	10	125	105	4	165	164
2	127	110	7	L46	36-	H	17	4	11	L45	2-	5	L36	12-
3	91	87-	8	76	67	0	L48	36-	12	66	72-	6	154	153-
4	56	50-	9	L49	16-	1	L49	42-	13	69	66	7	118	110
5	76	86	10	L51	22-	2	62	62	14	52	2	8	48	26-
6	43	32-	11	64	49	3	L52	22-	15	L54	55-	9	78	80-
7	57	48-	H	12	4	4	L53	31-	16	62	54	10	75	76

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
11	L49	3-	0	36	21	2	73	77-	4	118	120	5	136	137-
12	52	58-	1	109	110-	3	80	81	5	137	144-	6	116	110
13	54	59	2	113	113	4	L52	7	6	98	81	7	L46	7
H	6	5	3	L41	31	5	60	54-	7	64	60	8	118	117-
0	L29	4-	4	78	82-	H	14	5	8	117	119-	9	L52	50
1	152	161-	5	75	72	0	69	66-	9	80	75	10	54	16
2	119	118	6	L47	25	1	70	50	10	48	45	11	70	75-
3	38	21	7	91	93-	2	L52	18-	11	116	111-	12	L59	28
4	81	88-	8	71	54	3	64	59-	12	66	47	H	6	6
5	77	80	9	L53	10	4	L54	41	13	L57	18	0	139	150-
6	L40	18	10	77	67-	H	15	5	14	84	70-	1	98	105
7	77	76-	11	63	38	0	L51	14	H	3	6	2	L38	12
8	50	54	H	10	5	1	79	69-	0	162	222-	3	105	115-
9	L47	3	0	90	92	2	85	77	1	80	96	4	102	94
10	100	89-	1	L40	11-	3	55	8	2	59	63	5	50	50
11	57	52	2	101	102-	4	69	62-	3	166	190-	6	87	84-
12	L53	3	3	90	90	H	16	5	4	90	90	7	78	63
13	78	65-	4	24	1	0	76	60	5	L37	39	8	63	56
H	7	5	5	75	74-	1	L55	5-	6	102	103-	9	77	77-
0	73	73	6	78	81	2	56	44-	7	67	76	10	L57	38
1	L33	15	7	57	5-	H	17	5	8	64	64	11	L59	50
2	119	132-	8	53	47-	0	56	53-	9	96	89-	12	97	75-
3	86	90	9	86	70	H	0	6	10	L51	34	H	7	6
4	L38	18	H	11	5	0		349-	11	84	71	0	72	77
5	120	115-	0	89	93-	H	1	6	12	89	79-	1	94	108-
6	131	118	1	91	89	0		64	13	83	22	2	L40	42
7	L45	12	2	L45	40-	1		78-	H	4	6	3	73	80
8	81	81-	3	72	78-	2		6	0	92	107	4	157	164-
9	114	107	4	58	71	3	94	108	1	135	167-	5	L46	53
10	51	5-	5	L49	25-	4	130	154-	2	35	41	6	78	72
11	L53	50-	6	72	66-	5	L32	15	3	94	104	7	106	99-
12	61	70	7	75	62	6	81	64	4	135	148-	8	L53	42
H	8	5	8	55	16-	7	117	132-	5	L39	15	9	63	52
0	132	146-	H	12	5	8	L41	2	6	92	81	10	72	76-
1	155	150	0	L43	19	9	54	63	7	116	118-	H	8	6
2	L37	28-	1	51	70-	10	97	99-	8	47	29	0	L40	32
3	114	109-	2	102	100	11	L50	39	9	71	60	1	83	86
4	106	115	3	L48	18	12	64	57	10	98	98-	2	99	96-
5	L42	35-	4	79	77-	13	67	74-	11	L54	35	3	72	71
6	97	97-	5	78	77	14	65	38	12	71	54	4	L47	40
7	81	82	6	L53	20	15	60	38	H	5	6	5	99	97-
8	L49	12-	7	61	67-	H	2	6	0	34	43	6	L51	35
9	84	83-	8	56	51	0		68	1	116	128	7	L53	19
10	87	71	H	13	5	1	103	141	2	117	116-	8	55	60-
11	L55	11	0	52	62	2	94	119-	3	70	70	9	L58	24
H	9	5	1	L48	3	3	58	69	4	63	55	H	9	6

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
0	77	74-	H	14	6	8	58	65-	2	85	94	2	39	30-
1	L44	33	0	L57	47	9	L55	11	3	78	76-	3	L32	37-
2	L46	35	1	L58	52	10	66	64	4	L51	3	4	72	100
3	79	85-	H	15	6	11	L62	47-	5	90	86	5	48	26-
4	L50	44	0	L59	60-	12	L65	8-	6	106	93-	6	43	36-
5	64	54	1	L60	26	H	4	7	7	L60	3-	7	101	111
6	60	61-	H	16	6	0	70	84-	8	62	56	8	50	14-
7	L55	41	0	L62	10	1	L34	11	9	79	74-	9	66	48-
8	L58	36	1	70	61-	2	88	89	H	8	7	10	82	73
9	74	60-	H	1	7	3	69	81-	0	88	91	11	L61	28-
H	10	6	0		99-	4	L43	26	1	97	101-	12	71	37-
0	51	59	1		63	5	79	92	2	L50	21	H	2	8
1	123	129-	2	85	131	6	104	110-	3	102	84	0		74-
2	L48	39	3	78	93-	7	L51	20-	4	78	93-	1	47	76-
3	L51	35	4	L34	2	8	86	77	5	L57	27	2	62	85
4	118	122-	5	128	133	9	92	94-	6	66	73	3	71	81-
5	L54	38	6	81	89-	10	L61	11-	H	9	7	4	L39	40-
6	63	45	7	44	8-	11	63	67	0	L50	18-	5	86	98
7	83	83-	8	83	83	12	74	73-	1	73	74	6	65	64-
H	11	6	9	100	86-	H	5	7	2	75	81-	7	55	44-
0	54	65	10	L54	10-	0	118	146	3	L55	29-	8	102	96
1	71	66	11	92	85	1	124	142-	4	58	71	9	62	52-
2	81	85-	12	92	87-	2	L40	3	5	L59	59-	10	L60	21-
3	L53	46	H	2	7	3	127	132	H	10	7	11	69	77
4	L54	52	0		134	4	114	124-	0	53	64-	H	3	8
5	70	73-	1	85	120-	5	L48	22	1	L54	6	0	86	127
6	59	29	2	55	56-	6	121	116	2	98	85	1	44	65-
7	L60	18	3	139	153	7	102	91-	3	66	69-	2	L35	33-
H	12	6	4	120	124-	8	L57	19	4	L61	5-	3	82	110
0	96	95-	5	L40	3-	9	85	70	5	63	60	4	66	73-
1	L52	32	6	136	138	10	70	59-	H	11	7	5	50	49-
2	77	63	7	L47	74-	H	6	7	0	79	70	6	78	87
3	79	68-	8	50	10	0	L39	3-	1	58	72-	7	58	62-
4	64	42	9	108	115	1	96	100	2	L59	19	8	55	56-
5	59	46	10	79	78-	2	79	84-	3	69	68	9	L58	66
6	L62	54-	11	66	7-	3	L46	16-	H	12	7	10	61	47-
7	L63	38	12	62	67	4	69	67	0	L59	16-	H	4	8
H	13	6	H	3	7	5	93	78-	1	74	64	0	58	57-
0	L53	33	0		25-	6	L54	6-	2	70	75-	1	94	113
1	107	96-	1	90	94	7	70	60	H	13	7	2	L39	35-
2	L57	29	2	102	115-	8	L59	47-	0	62	53-	3	L42	40-
3	L58	25	3	L36	24-	9	62	5-	H	0	8	4	98	104
4	112	91-	4	57	75	10	65	67	0		224	5	L48	3
5	76	42	5	92	93-	H	7	7	H	1	8	6	57	59-
6	L64	20	6	L46	16-	0	65	49-	0		61-	7	94	85
7	80	65-	7	L50	44	1	L44	4-	1		107	8	L57	13-

TABLE 25. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
9	L61	33-	2	L56	24-									
H	5	8	3	58	68									
0	54	63-	4	L61	34-									
1	57	65-	5	L63	34-									
2	68	72	6	L65	59									
3	68	66-	7	L68	37-									
4	48	38-	8	L69	29-									
5	72	72	H	10	8									
6	61	50-	0	68	61-									
7	L57	19-	1	100	103									
8	L60	73	2	L60	43-									
9	L62	35-	3	L61	18-									
H	6	8	4	90	88									
0	96	116	5	L65	40-									
1	54	71-	6	L68	32-									
2	L46	26-	7	L70	71									
3	78	93	8	80	30-									
4	62	50-	H	11	8									
5	61	54-	0	65	50-									
6	64	64	1	L61	36-									
7	L60	45-	H	12	8									
8	L62	41-	0	62	67									
9	72	63	1	L64	25-									
H	7	8	H	13	8									
0	72	71-	0	L65	31-									
1	114	111	1	94	72									
2	L50	29-												
3	51	66-												
4	127	117												
5	L57	22-												
6	L60	54-												
7	76	83												
8	L65	34-												
H	8	8												
0	78	60-												
1	50	64-												
2	60	66												
3	L55	50-												
4	L57	33-												
5	L60	55												
6	L63	24-												
7	L65	30-												
8	L68	56												
H	9	8												
0	90	89												
1	L54	30-												

TABLE 26. STRUCTURE FACTORS FOR YTTRIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES $\leq$ AND K = 1.2)

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
H	1	0	12	36	25	1	122	134	5	36	31	8	40	20-
0		161-	13	L12	1	2	27	36-	H	12	0	9	132	127-
1	58	54	H	4	0	3	116	117-	0	50	40	10	68	65
2	52	44	0	117	111-	4	126	136	1	L30	20-	11	L33	5
3	46	48-	1	96	102	5	L31	21	2	L28	20-	12	30	33-
4	80	84	2	145	143-	6	93	90-	3	L26	11	13	L25	22
5	26	23-	3	L22	7-	7	63	73	4	29	28-	H	3	1
6	63	74-	4	69	63	8	38	34-	5	33	33-	0	166	148
7	229	234	5	95	97	9	50	54-	H	13	0	1	40	45-
8	L28	8	6	122	131-	10	61	56	0	L26	1	2	122	120
9	74	77-	7	60	45	H	8	0	1	54	55	3	L21	13
10	74	75	8	L32	18	0	L27	10-	2	L24	14-	4	34	28-
11	40	34-	9	L32	17-	1	148	153-	3	L20	11	5	70	66
12	L30	11-	10	43	41	2	102	98	4	48	56	6	62	53
13	L27	24	11	38	28-	3	53	52-	H	14	0	7	L31	25
14	29	29-	12	24	32-	4	L32	8-	0	34	32-	8	L33	28
H	2	0	13	17	15	5	53	51	1	33	37-	9	48	37-
0	111	110-	H	5	0	6	L31	6-	2	28	26	10	33	21-
1	208	219-	0	87	93	7	29	4	H	15	0	11	L07	1-
2	67	42-	1	138	131-	8	53	49	0	40	37	12	L27	5
3	133	125-	2	54	60	H	9	0	H	1	1	13	53	33-
4	25	17-	3	31	33-	0	94	90	0		150	H	4	1
5	123	128	4	52	52-	1	41	35-	1		281-	0	37	39
6	104	107-	5	99	102	2	L31	9	2	179	199-	1	37	42-
7	100	107-	6	57	54-	3	L32	13	3	35	38	2	59	42
8	124	135	7	L31	28	4	40	33-	4	L20	3-	3	24	35
9	87	97-	8	84	82	5	30	31-	5	219	208-	4	79	84-
10	40	13	9	47	51-	6	L28	27	6	56	51	5	74	71-
11	60	62	10	35	36	7	40	37-	7	L28	18	6	98	101
12	45	50-	11	33	32	8	31	33-	8	96	88-	7	79	69
13	30	28	H	6	0	H	10	0	9	89	74	8	55	52-
14	45	42	0	183	187	0	69	57-	10	L34	14	9	88	87
H	3	0	1	241	223-	1	120	113	11	76	71-	10	L32	14
0	274	310	2	52	52	2	40	33-	12	77	78	11	46	43-
1	193	204-	3	73	75	3	42	44	13	L28	13	12	63	58
2	231	215	4	36	35-	4	73	79	14	52	49-	H	5	1
3	120	131	5	72	72-	5	L28	28-	H	2	1	0	238	230-
4	155	155-	6	L31	6-	6	31	31-	0	180	208-	1	195	201
5	52	48	7	L32	17-	7	76	68	1	157	157	2	35	28-
6	52	37	8	50	51-	H	11	0	2	180	173	3	145	146-
7	47	34-	9	38	48	0	55	60-	3	166	164-	4	151	147
8	50	48-	10	27	26-	1	35	31-	4	195	191	5	L31	22-
9	L32	27	11	43	40-	2	L31	20	5	L24	25-	6	128	131-
10	40	19-	H	7	0	3	54	53-	6	171	177-	7	83	68
11	L29	24-	0	117	106-	4	L27	12-	7	48	48	8	34	38-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
9	32	35-	0	42	41	12	61	52	12	49	41	6	L33	6-
10	37	34	1	L34	20-	13	47	30-	H	5	2	7	L27	1
H	6	1	2	55	58-	14	L19	11	0	109	121	H	9	2
0	L24	18-	3	42	44	H	2	2	1	153	148	0	L30	13-
1	147	156-	4	L32	2	0	121	148	2	L24	5-	1	31	28-
2	63	60	5	L29	29-	1	202	226	3	93	94	2	27	8-
3	L29	27	6	47	42	2	95	109-	4	L28	6-	3	45	55-
4	L31	35-	H	11	1	3	68	67	5	77	75-	4	L31	16
5	L33	31	0	55	49-	4	118	114	6	137	132	5	30	34
6	L34	10	1	43	40	5	102	98-	7	36	41-	6	L30	18-
7	L34	22-	2	41	45-	6	66	56	8	82	64-	7	L23	18
8	L11	1-	3	39	40-	7	L29	13	9	L30	21	H	10	2
9	L30	7	4	L28	27	8	72	62-	10	L26	1	0	81	78
10	51	48-	5	25	29-	9	57	38	11	49	36-	1	108	111-
H	7	1	6	28	23-	10	L32	26	H	6	2	2	L32	20
0	L26	16-	H	12	1	11	94	86-	0	119	123-	3	L31	25
1	43	35	0	L33	27	12	L27	13	1	89	75	4	94	104-
2	81	85-	1	L32	22-	13	L22	8-	2	L26	17-	5	29	27
3	44	39	2	65	62	14	41	40-	3	105	105-	6	L25	19
4	L33	18	3	L27	25	H	3	2	4	120	118	7	46	44-
5	76	74-	4	46	43-	0	141	133-	5	41	35	H	11	2
6	89	82	5	40	39	1	L17	12	6	39	55-	0	62	60
7	L33	13	H	13	1	2	198	208	7	74	71	1	38	47
8	38	36-	0	L30	12	3	188	204-	8	30	33	2	L30	21-
9	74	71	1	35	9	4	73	71	9	L27	28-	3	L28	15
H	8	1	2	50	37-	5	95	96	10	L22	26	4	46	48
0	111	97-	3	48	41	6	58	65-	11	17	24	5	L21	23-
1	106	107	H	14	1	7	111	112	H	7	2	H	12	2
2	45	38-	0	L25	22-	8	79	66	0	67	62	0	66	57-
3	61	63-	1	L22	5	9	70	54-	1	36	42-	1	L29	6-
4	74	79	2	32	22-	10	31	33	2	L29	13-	2	46	48
5	48	43-	H	0	2	11	73	65	3	70	75	3	39	31-
6	53	54-	0		435-	12	L24	27-	4	176	188-	4	L22	16
7	30	34	H	1	2	H	4	2	5	32	35	5	24	24
8	L26	16-	0		61-	0	83	78	6	57	49	H	13	2
9	44	43-	1	L11	8-	1	232	241-	7	62	67-	0	L30	29
H	9	1	2	124	109-	2	37	39-	8	L30	15	1	73	67-
0	40	36	3	102	105	3	90	90	9	L23	26	H	1	3
1	65	56-	4	193	195-	4	147	157-	10	38	39-	0		84-
2	67	68	5	38	33-	5	61	56-	H	8	2	1	28	37
3	34	41	6	L25	9-	6	L30	42	0	L28	22	2	177	205
4	L34	35-	7	77	67-	7	98	89-	1	57	55	3	136	144-
5	L32	20	8	95	81-	8	L32	18-	2	L31	20	4	36	39-
6	38	36	9	L31	34	9	L31	38	3	76	69	5	167	169
7	57	47-	10	48	40-	10	73	66-	4	L32	15	6	125	118-
H	10	1	11	L31	5-	11	L25	1-	5	L32	20-	7	L24	2-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
8	L26	24	8	L27	18	6	34	44	9	29	44-	3	72	66-
9	92	82-	9	79	71-	7	30	26-	10	49	44	4	L28	20-
10	L27	14-	10	L23	16-	H	9	3	11	L26	11-	5	L29	33
11	43	38	11	33	27	0	55	54-	12	L22	18-	6	42	35-
12	77	68-	H	5	3	1	L27	26	13	16	19	7	L29	14
13	L19	21-	0	174	182	2	39	37-	H	2	4	8	43	43
14	24	33	1	111	119-	3	72	71-	0	90	109-	9	L23	28-
H	2	3	2	31	23	4	45	44	1	78	100-	10	26	16
0	127	137	3	132	137	5	L24	25-	2	L18	22	H	6	4
1	29	27-	4	94	95-	6	30	45-	3	108	113-	0	128	123
2	62	62-	5	37	32	7	42	43	4	L23	8	1	97	101-
3	152	151	6	135	134	H	10	3	5	74	72	2	L27	12
4	48	45-	7	50	53-	0	L27	29-	6	77	70-	3	76	73
5	L22	5	8	L26	35	1	L27	36	7	56	45-	4	L29	33-
6	168	167	9	56	51	2	68	61	8	91	85	5	59	56-
7	L26	11	10	21	29-	3	44	32-	9	41	52-	6	L29	16
8	L27	2	H	6	3	4	L23	10	10	L27	11	7	L27	30-
9	142	142	0	L21	13-	5	29	25	11	55	50	8	34	34-
10	52	50-	1	32	37	H	11	3	H	3	4	9	L19	35
11	24	9-	2	24	31-	0	27	30	0	104	116	H	7	4
12	55	51	3	80	71-	1	53	56-	1	65	72-	0	98	86-
13	L16	26-	4	L26	11	2	L24	35	2	L20	31	1	106	111
H	3	3	5	50	44-	3	L22	26	3	82	84	2	L29	4-
0	79	95-	6	39	34-	4	L19	28-	4	98	96-	3	79	81-
1	22	19-	7	26	21	H	12	3	5	L27	35-	4	107	118
2	91	101-	8	L24	14-	0	35	35-	6	55	48	5	L29	14
3	73	69-	9	L21	16-	1	39	37	7	65	57-	6	60	55-
4	L21	2	10	41	40	2	41	46-	8	57	50-	7	55	64
5	71	59-	H	7	3	3	23	33-	9	L28	27	8	38	23-
6	62	60-	0	L23	9	4	53	53	10	L25	39-	9	20	33-
7	L27	27-	1	L24	15	H	13	3	H	4	4	H	8	4
8	L27	30-	2	97	95	0	L21	13-	0	39	44-	0	58	54-
9	L27	17	3	53	49-	1	L19	9-	1	99	99	1	79	83-
10	L25	25	4	47	37	2	39	34	2	23	34-	2	29	29
11	L22	3-	5	67	56	H	0	4	3	L25	5	3	41	45-
12	L18	8-	6	72	64-	0		489	4	75	75	4	L28	10-
13	30	30	7	L24	8	H	1	4	5	77	79	5	L26	12
H	4	3	8	L21	17	0		71-	6	65	69-	6	L24	1
0	63	67-	9	42	44-	1	79	98	7	57	50	7	L20	10-
1	L18	1	H	8	3	2	L16	13	8	L28	24	H	9	4
2	88	77	0	70	62	3	L19	9	9	L26	10-	0	76	75
3	103	100-	1	105	96-	4	66	74	10	32	37	1	L29	11-
4	94	98	2	L27	34	5	24	6-	H	5	4	2	L29	11
5	58	57	3	47	51	6	L26	13-	0	62	50-	3	28	24
6	131	121-	4	78	74-	7	131	127	1	61	66-	4	L26	22-
7	27	18-	5	26	38	8	L29	23	2	L25	15	5	L23	18-

TABLE 26. CONTINUED

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
6	L19	26												
7	17	28-												
H	10	4												
0	70	66-												
1	85	94												
2	L27	33-												
3	L25	18												
4	61	68												
H	11	4												
0	56	46-												
1	L26	17-												
2	L24	3												
3	21	31-												
H	12	4												
0	35	31												
1	L22	6-												
H	13	4												
0	66	14-												
1	46	48												

TABLE 27. STRUCTURE FACTORS FOR PRASEODYMIUM ETHYLSULFATE NONAHYDRATE (L IMPLIES ≤ AND K = 1.2)

H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c	H	KF_o	KF_c
H	1	0	7	84	79-	1	269	277-	3	84	80	7	77	92
0		201-	8	83	87-	2	L38	15	4	78	61-	8	83	45-
1		132	9	93	91	3	149	169	5	80	67-	H	14	0
2		2	10	61	56-	4	78	78-	6	94	91	0	73	75-
3	87	95-	11	66	63-	5	122	118-	7	75	80-	1	75	72-
4	173	182	12	81	93	6	51	57	8	71	66-	2	97	89
5	70	64-	13	L60	25-	7	62	55-	9	93	98	3	L63	29-
6	122	118-	14	74	81-	8	89	93-	H	10	0	4	68	52-
7	294	329	15	98	104	9	121	128	0	101	90-	5	L67	58
8	L42	32-	H	4	0	10	L58	54-	1	172	189	6	L69	4-
9	116	111-	0	167	159-	11	79	80-	2	90	73-	7	L71	38-
10	133	146	1	183	204	12	90	99	3	52	16	H	15	0
11	77	67-	2	183	187-	13	L67	30-	4	149	168	0	98	97
12	L54	41-	3	70	63-	14	L69	42-	5	70	66-	1	67	49-
13	91	89	4	146	162	15	87	96	6	68	70-	2	72	58-
14	77	67-	5	107	86	H	7	0	7	123	138	3	71	69
15	73	64-	6	170	179-	0	177	171-	8	L63	52-	4	68	41-
16	94	87	7	131	124	1	187	215	H	11	0	5	74	52-
17	80	48-	8	L48	15-	2	70	77-	0	101	91-	6	L72	53
18	75	21-	9	51	54-	3	160	167-	1	60	63-	7	80	44-
H	2	0	10	114	116	4	186	221	2	85	90	H	16	0
0		147-	11	64	57-	5	L48	19-	3	94	89-	0	L64	10-
1		260-	12	72	67-	6	147	140-	4	57	46-	1	99	107
2		40	13	70	75	7	136	153	5	90	90	2	67	49-
3	195	202-	14	79	53-	8	100	78-	6	L61	27-	3	L69	16-
4	88	73-	15	85	54-	9	94	92-	7	L63	21-	4	76	72
5	207	224	H	5	0	10	110	118	8	80	68	5	72	33-
6	141	141-	0	63	45	11	63	56-	H	12	0	H	17	0
7	144	149-	1	187	187-	H	8	0	0	108	107	0	L67	39-
8	196	215	2	145	151	0	70	57-	1	63	53-	1	68	54-
9	147	152-	3	75	69-	1	186	195-	2	70	63-	H	18	0
10	L50	24-	4	110	107-	2	173	179	3	72	70	0	90	80
11	117	129	5	173	173	3	110	103-	4	70	60-	1	75	38-
12	95	93-	6	107	106-	4	L48	33-	5	86	71-			
13	L57	1	7	L48	12	5	121	123	6	L64	60			
14	111	110	8	159	171	6	54	47-	7	L66	43-			
15	72	65-	9	85	85-	7	L55	27-	8	68	43-			
H	3	0	10	L56	9	8	116	117	H	13	0			
0		400	11	94	94	9	L60	40-	0	57	33-			
1	230	244-	12	L61	23-	10	L63	12-	1	120	138			
2	214	184	13	L64	5-	11	74	64	2	L58	49-			
3	204	226	14	71	55	H	9	0	3	L60	22			
4	184	183-	15	L70	22-	0	147	168	4	107	122			
5	L38	3	H	6	0	1	93	72-	5	64	36-			
6	126	122	0	256	273	2	L47	15-	6	L67	34-			